MOLAR HEAT CAPACITIES DESCRIBED MORE ACCURATELY

By

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The heat capacity of chemicals is very important for research work and engineering design in the chemical industries. Curve fitting experimental C_p^0 values for gases using a polynomial form:

$$C_p^0 = a + bT + cT^2 + dT^3$$

has been shown to describe heat capacity data for more than 700 compounds over the range from 273 to 1000 K usually within an average percentage error of 0.1%. All data are given both in calories and joules as energy units.

The equilibrium constant of a chemical reaction can be calculated for any temperature from the standard enthalpies of formation ($\Delta H_{f,298}^0$) the standard entropies (S_{298}^0) and the molar heat capacities (C_p^0) of the compounds. The basic equation used in the calculation is

$$\ln K_p = \frac{\Delta S_T^0}{R} - \frac{\Delta H_T^0}{RT}$$

where the reaction enthalpy and reaction entropy are calculated from the standard state reaction enthalpy and reaction entropy by the equations

$$\Delta H_T^0 = \Delta H_{298}^0 + \int_{298}^{T} \Delta C_p^0 \, dT \tag{1}$$

and

$$\Delta S_T^0 = \Delta S_{298}^0 + \int_{298}^{T} \frac{\Delta C_p}{T} \, dT \tag{2}$$

ΔC_p^0 can be approximated by an average value, easily calculable from the known C_p^0 data taken from detailed tables, but the error committed is not always negligible.

Alternatively, empirical molar heat capacity functions may be used. They are generally given [1—7] in one of the forms:

$$C_p^0 = a + bT + cT^2$$

$$C_p^0 = a + bT + cT^{-2}$$

$$C_p^0 = a + bT + cT^2 + dT^3 \tag{3}$$

$$C_p^0 = a + be^{-c/T^n} \tag{4}$$

The last two formulae are known to describe the molar heat capacities of ideal gases to a precision of 0.5 per cent on the average in the temperature range of 298—1500 K. The polynomial forms have the advantage of giving a concise form of representation compared to the rather extensive tabular one and a simple way of calculation of the integrals in eqs. (1) and (2), which can be performed by a desk computer or even by hand; this is a considerable advantage in engineering and educational usage where single problems are to be solved rapidly [8, 9].

Equation (3) has been shown [3, 4, 7] to be less adequate than eq. (4) for describeing the C_p^0 values at both high and very low temperatures. On the other hand, it should be emphasized that our descriptions are aimed at calculating the enthalpy, entropy and Gibbs energy functions of compounds or reactions, and the exponential form has no specific advantage in this respect [5]. The unquestionable advantage of eq. (4) permitting extrapolations to very high and low temperatures can be useful in specific applications; however, most chemical reactions are studied between room temperature and 1000 K. Furthermore, the thermal instability of many of the compounds has been emphasized [5].

Considering all these facts, it was decided to make an extended collection of high—precision data of correlation coefficients calculated for a great number of compounds and radicals. Equation (3) was chosen for the calculation of correlation constants, but the error of approximation was decreased by calculating them for the temperature range of 298—1000 K instead of 298—1500 K. The restriction in the temperature range decreased the relative error of calculation in eq. (3). The computations were mostly based on the detailed and critical C_p^0 values published in the excellent book by STULL, WESTRUM and SINKE [10]; C_p^0 values of the radicals are taken from ref. [11].

The correlation constants of eq. (3), together with the $\Delta H_{f,298}^0$ and S_{298}^0 data, are collected in Table I for a great number of inorganic and organic compounds and some radicals.

As it may be desirable to have the results in SI units, too, all data are given using both calories and joules as energy units (symbols *C* and *J* in Table I). In order to avoid clerical errors the C_p^0 values were recalculated from eq. (3) and compared with the experimental data. The average and maximum errors are given in the last two columns of Table I.

In order to demonstrate the capability of the present choice of deriving correlation constants of high precision, C_p^0 correlation constants of eq. (3) have been computed from detailed C_p^0 tables [12] for both the temperature ranges of 298—1000 K and 298—1500 K (Table II). (No molar heat capacities for temperatures higher than 1000 K are to be found in ref [10]).

Table I.

Thermodynamic data of various species in the gas phase

INORGANIC COMPOUNDS

No.	Compound		ΔH_f^0 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
1	Carbon	C	0.00	1.36	−11.4860	1.32689	−8.91844	1.93701	0.08	0.198
		J	0.00	5.69	−48.0575	5.55169	−37.3148	8.10446	at 400 K	
2	Hydrogen	C	0.00	31.21	64.5042	0.23951	−3.60627	1.98299	0.09	0.225
		J	0.00	130.58	269.885	1.00210	−15.0886	8.29686	at 400 K	
3	Bromine [a]	C	0.00	36.38	80.8679	0.26881	−2.84643	1.08333	0.01	0.027
		J	0.00	152.21	338.351	1.12470	−11.9095	4.53266	at 500 K	
4	Chlorine	C	0.00	53.29	64.3097	0.80670	−9.19273	3.65709	0.08	0.190
		J	0.00	222.97	269.071	3.37525	−38.4624	15.3013	at 400 K	
5	Fluorine	C	0.00	48.45	55.4518	0.87342	−8.26923	2.87644	0.02	0.037
		J	0.00	202.71	232.010	3.65437	−34.5984	12.0350	at 900 K	
6	Iodine [b]	C	0.00	27.76	86.1816	0.10480	−0.94762	0.34259	0.01	0.005
		J	0.00	116.15	360.584	0.43848	−3.96484	1.43341	at 900 K	
7	Nitrogen	C	0.00	45.77	73.5693	−0.28143	5.70963	−2.43682	0.02	0.032
		J	0.00	191.50	307.814	−1.17751	23.8891	−10.1956	at 400 K	
8	Oxygen	C	0.00	49.00	67.1136	−0.00088	4.16903	−2.54445	0.11	0.250
		J	0.00	205.02	280.803	−0.00368	17.4432	−10.6460	at 400 K	
9	Hydrogen bromide	C	−8.66	47.44	72.8295	−0.20953	3.87271	−1.37929	0.03	0.085
		J	−36.23	198.49	304.718	−0.87669	16.2034	−5.77096	at 298 K	
10	Cyanogen bromide	C	43.35	59.07	78.6815	1.47942	−14.5492	5.54065	0.13	0.317
		J	181.38	247.15	329.203	6.18989	−60.8738	23.1821	at 400 K	
11	Cyanogen chloride	C	31.60	56.28	69.4893	1.70429	−16.7541	6.33739	0.16	0.426
		J	132.21	235.48	290.743	7.13074	−70.0991	26.5156	at 400 K	
12	Phosgene	C	−52.80	67.82	67.0860	3.24979	−32.8057	12.1067	0.12	0.304
		J	−220.92	283.76	280.688	13.5971	−137.259	50.6546	at 400 K	
13	Carbonyl fluoride	C	−153.00	61.84	32.3268	3.53198	−30.7328	9.97596	0.04	0.063
		J	−640.15	258.74	135.255	14.7778	−128.586	41.7394	at 400 K	
14	Hydrogen cyanide	C	31.20	48.21	52.2084	1.44760	−11.8432	4.33510	0.10	0.279
		J	130.54	201.71	218.440	6.05677	−49.5521	18.1381	at 400 K	
15	Cyanogen iodide	C	53.80	61.33	89.3035	1.18558	−11.4784	4.42436	0.10	0.253
		J	225.10	256.60	373.645	4.96046	−48.0255	18.5115	at 400 K	
16	Carbon monoxide	C	−26.42	47.30	73.7126	−0.30674	6.66606	−3.03653	0.05	0.100
		J	−110.54	197.90	308.413	−1.28339	27.8908	−12.7048	at 600 K	
17	Carbonyl sulfide	C	−33.08	55.32	52.6321	2.08053	−19.3731	6.93582	0.11	0.279
		J	−138.41	231.46	220.213	8.70493	−81.0572	29.0195	at 400 K	
18	Carbon dioxide	C	−94.05	51.07	47.2691	1.75324	−13.3815	4.09619	0.04	0.091
		J	−393.51	213.68	197.774	7.33555	−55.9880	17.1385	at 400 K	
19	Carbon disulfide	C	27.98	56.83	65.5346	1.94088	−18.3063	6.38265	0.08	0.199
		J	117.07	237.78	274.196	8.12064	−76.5935	26.7050	at 400 K	
20	Cyanogen	C	73.84	57.90	84.9890	2.24759	−20.0032	7.29535	0.13	0.300
		J	308.95	242.25	355.594	9.40392	−83.6932	30.5237	at 400 K	
21	Carbon suboxide	C	−22.38	66.05	83.1497	3.29189	−26.0099	8.17586	0.25	0.425
		J	−93.64	276.35	347.898	13.7733	−108.826	34.2078	at 400 K	
22	Acetylene-dicarbonitrile	C	127.50	69.31	114.537	3.99329	−35.3041	12.5643	0.13	0.344
		J	533.46	289.99	479.223	16.7079	−147.712	52.5688	at 400 K	
23	Perchloryl fluoride	C	−6.49	66.65	29.4200	5.71878	−56.1227	19.8932	0.10	0.217
		J	−27.15	278.86	123.093	23.9273	−234.818	83.2332	at 400 K	

[a] Ideal gas state from 332.62 K [b] Ideal gas state from 458.39 K.

Table I. (cont.)

No.	Compound		ΔH_f^0 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
24	Hydrogen chloride	C	−22.06	44.64	72.3371	−0.17173	2.97529	−0.93086	0.03	0.097
		J	−92.30	186.77	302.658	−0.71851	12.4486	−3.89472		at 400 K
25	Nitrosyl chloride	C	12.57	62.53	81.3383	1.07282	−8.04210	2.45402	0.05	0.129
		J	52.59	261.63	340.319	4.48866	−33.6481	10.2676		at 400 K
26	Nitryl chloride	C	3.12	65.01	57.7747	3.05042	−26.8917	8.81780	0.05	0.135
		J	13.05	272.00	241.729	12.7629	−112.515	36.8937		at 400 K
27	Thionyl chloride	C	−50.60	73.23	102.323	2.63976	−27.9930	10.5586	0.10	0.246
		J	−211.71	306.39	428.121	11.0448	−117.123	44.1772		at 400 K
28	Sulfuryl chloride	C	−85.40	74.37	96.3610	4.12216	−45.3315	17.5003	0.14	0.341
		J	−357.31	311.16	403.174	17.2471	−189.667	73.2212		at 400 K
29	Sulfur monochloride	C	−4.66	76.35	122.678	2.51616	−30.0199	12.2213	0.13	0.320
		J	−19.50	319.45	513.286	10.5276	−125.603	51.1339		at 400 K
30	Hydrogen fluoride	C	−64.80	41.51	69.4116	0.01579	−0.48543	0.59797	0.03	0.073
		J	−271.12	173.68	290.418	0.06606	−2.03103	2.50189		at 400 K
31	Nitrosyl fluoride	C	−15.70	59.27	65.6311	1.43947	−12.0657	3.89199	0.04	0.098
		J	−65.69	247.99	274.600	6.02273	−50.4828	16.2841		at 400 K
32	Nitryl fluoride	C	−19.00	62.24	42.3348	3.39036	−30.1014	9.95429	0.07	0.178
		J	−79.50	260.41	177.128	14.1852	−125.944	41.6487		at 400 K
33	Sulfur tetrafluoride	C	−174.10	69.58	29.5760	6.76422	−74.8376	28.9088	0.21	0.500
		J	−728.43	291.12	123.746	28.3015	−313.121	120.954		at 400 K
34	Hydrogen iodide	C	6.30	49.35	73.7285	−0.29777	6.27655	−2.75178	0.01	0.017
		J	26.36	206.48	308.480	−1.24588	26.2611	−11.5134		at 800 K
35	Hydrogen nitrate	C	−32.02	63.68	24.3115	4.47573	−36.5813	11.3499	0.03	0.099
		J	−133.97	266.44	101.720	18.7264	−153.056	47.4880		at 700 K
36	Water	C	−57.80	45.11	79.1209	−0.08050	4.52165	−1.78026	0.04	0.117
		J	−241.84	188.74	331.042	−0.33683	18.9186	−7.44860		at 400 K
37	Hydrogen peroxide	C	−32.53	55.66	43.7848	2.63807	−24.3565	8.62144	0.05	0.086
		J	−136.11	232.88	183.196	11.0377	−101.908	36.0721		at 900 K
38	Sulfuric acid	C	−194.45	37.49	87.3176	12.9904	−190.725	101.733	0.04	0.055
		J	−813.58	156.86	365.337	54.3518	−797.995	425.650		at 298 K
39	Hydrogen sulfide	C	−4.82	49.18	76.2736	0.03430	5.80808	−2.80972	0.02	0.047
		J	−20.17	205.77	319.129	0.14351	24.3010	−11.7559		at 400 K
40	Ammonia	C	−10.92	46.03	65.2275	0.56910	4.07713	−2.82965	0.11	0.328
		J	−45.69	192.59	272.912	2.38113	17.0587	−11.8393		at 400 K
41	Hydrazine	C	22.75	57.41	17.1396	4.80640	−43.4577	16.0157	0.26	0.591
		J	95.19	240.20	71.7120	20.1099	−181.827	67.0094		at 400 K
42	Nitric oxide	C	21.60	50.35	76.5366	−0.39187	8.41319	−4.03457	0.10	0.196
		J	90.37	210.66	320.229	−1.63958	35.2008	−16.8806		at 400 K
43	Nitrogen dioxide	C	8.09	57.35	60.4622	1.04283	−3.21450	−0.63769	0.08	0.232
		J	33.85	239.95	252.974	4.36319	−13.4495	−2.66808		at 400 K
44	Nitrous oxide	C	19.49	52.56	51.6269	1.73826	−13.8008	4.36984	0.05	0.125
		J	81.55	219.91	216.007	7.27287	−57.7428	18.2834		at 400 K
45	Sulfur dioxide	C	−70.95	59.30	59.1923	1.49703	−10.3565	2.48316	0.06	0.185
		J	−296.85	248.11	247.660	6.26356	−43.3316	10.3895		at 400 K
46	Ozone	C	34.00	57.05	43.9309	2.20263	−19.8425	6.46368	0.05	0.120
		J	142.26	238.70	183.806	9.21580	−83.0212	27.0440		at 400 K
47	Sulfur trioxide	C	−94.47	61.19	33.4938	3.77767	−31.3285	9.95898	0.06	0.177
		J	−395.26	256.02	140.138	15.8058	−131.078	41.6683		at 400 K

Table I. (cont.)

HYDROCARBONS

No.	Compound		ΔH_f^0 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
101	Methane	C	−17.89	44.52	60.6064	0.40338	17.0402	−9.75829	0.23	0.676
		J	−74.85	186.27	253.576	0.16877	71.2959	−40.8286		at 400 K
102	Ethane	C	−20.24	54.85	19.5639	3.85853	−9.56761	−1.66412	0.15	0.465
		J	−84.68	229.49	81.8553	16.1441	−40.0309	−6.96267		at 400 K
103	Propane	C	−24.82	64.51	−12.7422	7.41401	−39.3353	8.28374	0.10	0.346
		J	−103.85	269.91	−53.3136	31.0202	−164.579	34.6591		at 400 K
104	Butane	C	−30.15	74.12	−4.24611	9.24822	−46.1826	8.32206	0.11	0.376
		J	−126.15	310.12	−17.7657	38.6945	−193.228	34.8195		at 400 K
105	2-Methylpropane	C	−32.15	70.42	−25.9145	10.2886	−60.1083	14.1979	0.08	0.282
		J	−134.52	294.64	−108.426	43.0473	−251.493	59.4037		at 400 K
106	Pentane	C	−35.00	83.40	−8.09997	11.5888	−60.1667	11.6097	0.11	0.359
		J	−146.44	348.95	−33.8903	48.4876	−251.737	48.5748		at 400 K
107	2-Methylbutane	C	−36.92	82.12	−26.9545	12.3338	−68.8008	15.2498	0.10	0.322
		J	−154.47	343.59	−112.778	51.6047	−287.8622	63.8052		at 400 K
108	2,2-Dimethyl-propane	C	−39.67	73.23	−48.2254	13.7538	−87.0097	22.0712	0.10	0.355
		J	−165.98	306.39	−201.775	57.5459	−364.049	92.3459		at 400 K
109	Hexane	C	−39.96	92.83	−2.87839	13.4878	−68.2091	12.4964	0.13	0.329
		J	−167.19	388.40	−12.0432	56.4332	−285.387	52.2847		at 600 K
110	2-Methylpentane	C	−41.66	90.95	−30.4564	15.0698	−90.4900	22.0076	0.11	0.371
		J	−174.31	380.53	−127.429	63.0522	−378.610	92.0796		at 400 K
111	3-Methylpentane	C	−41.02	90.77	−11.3403	13.9165	−74.1050	14.9306	0.11	0.369
		J	−171.63	379.78	−47.4477	58.2267	−310.055	62.4697		at 400 K
112	2,2-Dimethyl-butane	C	−44.35	85.62	−50.4135	15.6393	−93.5182	21.7576	0.20	0.559
		J	−185.56	358.23	−210.930	65.4349	−391.280	91.0338		at 400 K
113	2,3-Dimethyl-butane	C	−42.49	87.42	−39.2145	14.9389	−84.9397	18.5425	0.09	0.301
		J	−177.78	365.76	−164.074	62.5044	−355.388	77.5820		at 400 K
114	Heptane	C	−44.88	102.27	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−187.7	427.90	−56.0573	67.6862	−363.822	74.0097		at 400 K
115	2-Methylhexane	C	−46.59	100.38	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−194.93	419.99	−56.0573	67.6862	−363.822	74.0097		at 400 K
116	3-Methylhexane	C	−45.96	101.37	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−192.30	424.13	−56.0573	67.6862	−363.822	74.0097		at 400 K
117	3-Ethylpentane	C	−45.33	98.35	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−189.66	411.50	−56.0573	67.6862	−363.822	74.0097		at 400 K
118	2,2-Dimethyl-pentane	C	−49.27	93.90	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−206.15	392.88	−56.0573	67.6862	−363.822	74.0097		at 400 K
119	2,3-Dimethyl-pentane	C	−47.62	98.96	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−199.24	414.05	−56.0573	67.6862	−363.822	74.0097		at 400 K
120	2,4-Dimethyl-pentane	C	−48.28	94.80	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−202.00	396.64	−56.0573	67.6862	−363.822	74.0097		at 400 K
121	3,3-Dimethyl-pentane	C	−48.17	95.53	−13.3980	16.1774	−86.9557	17.6888	0.10	0.334
		J	−201.54	399.70	−56.0573	67.6862	−363.822	74.0097		at 400 K
122	2,2,3-Trimethyl-butane	C	−48.95	91.61	−62.8126	18.3781	−111.747	26.5196	0.13	0.429
		J	−204.81	383.30	−262.808	76.8941	−467.550	110.958		at 400 K
123	Octane	C	−49.82	111.55	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−208.45	466.73	−74.5327	77.7318	−428.230	91.6466		at 400 K
124	2-Methylheptane	C	−51.50	108.81	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−215.48	455.26	−74.5327	77.7318	−428.230	91.6467		at 400 K

Table I. (1. cont.)

No.	Compound		ΔH_f^0 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
125	3-Methylheptane	C	−50.82	110.32	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−212.63	461.58	−74.5327	77.7318	−428.230	91.6466	at 400 K	
126	4-Methylheptane	C	−50.69	108.35	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−212.09	453.34	−74.5327	77.7318	−428.230	91.6466	at 400 K	
127	3-Ethylhexane	C	−50.40	109.51	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−210.87	458.19	−74.5327	77.7318	−428.230	91.6466	at 400 K	
128	2,2-Dimethyl-hexane	C	−53.71	103.06	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−224.72	431.20	−74.5327	77.7318	−428.230	91.6466	at 400 K	
129	2,3-Dimethyl-hexane	C	−51.13	106.11	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−213.93	443.96	−74.5327	77.7318	−428.230	91.6466	at 400 K	
130	2,4-Dimethyl-hexane	C	−52.44	106.51	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−219.41	445.64	−74.5327	77.7318	−428.230	91.6466	at 400 K	
131	2,5-Dimethyl-hexane	C	−53.21	104.93	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−222.63	439.03	−74.5327	77.7318	−428.230	91.6466	at 400 K	
132	3,3-Dimethyl-hexane	C	−52.61	104.70	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−220.12	438.06	−74.5327	77.7318	−428.230	91.6466	at 400 K	
133	3,4-Dimethyl-hexane	C	−50.91	107.15	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−213.01	448.32	−74.5327	77.7318	−428.230	91.6466	at 400 K	
134	3-Ethyl-2--methylpentane	C	−50.48	105.43	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−211.21	441.12	−74.5327	77.7318	−428.230	91.6466	at 400 K	
135	3-Ethyl-3--methylpentane	C	−51.38	103.48	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−214.97	432.96	−74.5327	77.7318	−428.230	91.6466	at 400 K	
136	2,2,3-Trimethyl-pentane	C	−52.61	101.62	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−220.12	425.18	−74.5327	77.7318	−428.230	91.6466	at 400 K	
137	2,2,4-Trimethyl-pentane	C	−53.57	101.15	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−224.14	423.21	−74.5327	77.7318	−428.230	91.6466	at 400 K	
138	2,3,3-Trimethyl-pentane	C	−51.73	103.14	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−216.44	431.54	−74.5327	77.7318	−428.230	91.6466	at 400 K	
139	2,3,4-Trimethyl-pentane	C	−51.97	102.31	−17.8137	18.5783	−102.349	21.9041	0.10	0.344
		J	−217.44	428.07	−74.5327	77.7318	−428.230	91.6466	at 400 K	
140	2,2,3,3-Tetra-methylbutane	C	−53.99	93.06	−106.691	23.3942	−160.159	43.4570	0.09	0.305
		J	−225.89	389.36	−446.394	97.8813	−670.106	181.824	at 400 K	
141	Nonane	C	−54.74	120.86	−19.9958	20.8426	−115.192	24.6206	0.10	0.335
		J	−229.03	505.68	−83.6626	87.2055	−481.963	103.013	at 400 K	
142	2-Methyloctane	C	−56.45	118.52	8.65972	20.0906	−106.837	21.0212	0.12	0.335
		J	−236.19	495.89	36.2323	84.0590	−447.008	87.9526	at 400 K	
143	3-Methyloctane	C	−55.77	119.90	−28.2415	21.3603	−121.689	26.8737	0.11	0.303
		J	−233.34	501.66	−118.162	89.3715	−509.147	112.440	at 400 K	
144	4-Methyloctane	C	−55.77	119.90	−28.2415	21.3603	−121.689	26.8737	0.11	0.303
		J	−233.34	501.66	−118.162	89.3715	−509.147	112.440	at 400 K	
145	3-Ethylheptane	C	−55.08	118.52	−65.1427	22.6300	−136.541	32.7263	0.10	0.271
		J	−230.45	495.89	−272.557	94.6841	−571.286	136.927	at 400 K	
146	4-Ethylheptane	C	−55.08	118.52	−65.1427	22.6300	−136.541	32.7263	0.10	0.271
		J	−230.45	495.89	−272.557	94.6841	−571.286	136.927	at 400 K	
147	2,2-Dimethyl-heptane	C	−59.00	113.07	−44.3373	22.8410	−142.561	35.8395	0.12	0.383
		J	−246.86	473.08	−185.507	95.5666	−596.476	149.952	at 400 K	
148	2,3-Dimethyl-heptane	C	−56.32	116.79	−50.8233	22.2259	−132.231	31.0871	0.08	0.192
		J	−235.64	488.64	−212.645	92.9931	−553.254	130.069	at 400 K	
149	2,4-Dimethyl-heptane	C	−57.48	116.79	−85.9365	23.3957	−145.193	35.9011	0.08	0.149
		J	−240.50	488.65	−359.558	97.8874	−607.489	150.210	at 400 K	

Table 1. (2. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
150	2,5-Dimethyl-heptane	C	−57.48	116.79	−85.9365	23.3957	−145.193	35.9011	0.08	0.149
		J	−240.50	488.65	−359.558	97.8874	−607.489	150.210		at 400 K
151	2,6-Dimethyl-heptane	C	−58.17	114.03	−49.0353	22.1259	−130.342	30.0486	0.08	0.183
		J	−243.38	477.10	−205.164	92.5749	−545.350	125.723		at 400 K
152	3,3-Dimethyl-heptane	C	−57.74	115.25	−81.2385	24.1107	−157.413	41.6920	0.11	0.351
		J	−241.58	482.21	−339.902	100.879	−658.615	174.439		at 400 K
153	3,4-Dimethyl-heptane	C	−55.63	117.48	−87.7245	23.4956	−147.082	36.9397	0.08	0.158
		J	−232.76	491.54	−367.039	98.3057	−615.393	154.556		at 400 K
154	3,5-Dimethyl-heptane	C	−56.79	116.10	−122.838	24.6654	−160.045	41.7537	0.07	0.143
		J	−237.61	485.76	−513.953	103.200	−669.628	174.697		at 298 K
155	4,4-Dimethyl-heptane	C	−57.74	113.87	−81.2385	24.1107	−157.413	41.6920	0.11	0.351
		J	−241.58	476.43	−339.902	100.879	−658.615	174.439		at 400 K
156	3-Ethyl-2-methyl-hexane	C	−55.63	116.79	−87.7245	23.4956	−147.082	36.9397	0.08	0.158
		J	−232.76	488.65	−367.039	98.3057	−615.393	154.556		at 400 K
157	4-Ethyl-2-methyl-hexane	C	−56.79	115.41	−122.838	24.6654	−160.045	41.7537	0.07	0.143
		J	−237.61	482.88	−513.953	103.200	−669.628	174.697		at 298 K
158	3-Ethyl-3-methyl-hexane	C	−56.48	115.25	−118.140	25.3804	−172.264	47.5446	0.10	0.319
		J	−236.31	482.21	−49.4296	106.192	−720.754	198.926		at 400 K
159	3-Ethyl-4-methyl-hexane	C	−54.94	116.79	−124.626	24.7653	−161.934	42.7922	0.08	0.145
		J	−229.87	488.65	−521.434	103.618	−677.532	179.043		at 298 K
160	2,2,3-Trimethyl-hexane	C	−57.65	111.34	−103.820	24.9763	−167.955	45.9054	0.08	0.241
		J	−241.21	465.85	−434.384	104.501	−702.722	192.068		at 400 K
161	2,2,4-Trimethyl-hexane	C	−58.13	111.34	−138.934	26.1460	−180.9170	50.7194	0.08	0.200
		J	−243.22	465.85	−581.298	109.395	−756.957	212.210		at 400 K
162	2,2,5-Trimethyl-hexane	C	−60.71	109.96	−102.032	24.8763	−166.065	44.8669	0.08	0.233
		J	−254.01	460.07	−426.903	104.082	−694.818	187.723		at 400 K
163	2,3,3-Trimethyl-hexane	C	−57.08	112.14	−103.820	24.9762	−167.954	45.9053	0.08	0.241
		J	−238.82	469.19	−434.382	104.500	−702.719	192.068		at 400 K
164	2,3,4-Trimethyl-hexane	C	−56.18	114.37	−110.306	24.3612	−157.624	41.1531	0.07	0.129
		J	−235.06	478.52	−461.522	101.927	−659.499	172.185		at 298 K
165	2,3,5-Trimethyl-hexane	C	−58.03	112.30	−108.518	24.2612	−155.734	40.1145	0.07	0.127
		J	−242.80	469.86	−454.039	101.509	−651.593	167.839		at 298 K
166	2,4,4-Trimethyl-hexane	C	−57.56	112.14	−138.934	26.1460	−180.917	50.7195	0.08	0.200
		J	−240.83	469.19	−581.298	109.395	−756.957	212.210		at 400 K
167	3,3,4-Trimethyl-hexane	C	−56.39	113.52	−140.722	26.2460	−182.806	51.7580	0.08	0.208
		J	−235.94	474.97	−588.779	109.813	−764.861	216.555		at 400 K
168	3,3-Diethyl-pentane	C	−55.44	110.31	−155.041	26.6502	−187.116	53.3971	0.09	0.287
		J	−231.96	461.54	−648.691	111.504	−782.893	223.413		at 400 K
169	3-Ethyl-2,2-dimethylpentane	C	−56.96	109.96	−130.886	25.8408	−178.232	50.0362	0.07	0.169
		J	−238.32	460.07	−547.628	108.118	−745.725	209.352		at 400 K
170	3-Ethyl-2,3--dimethylpentane	C	−55.82	112.14	−140.722	26.2460	−182.806	51.7580	0.08	0.208
		J	−233.55	469.19	−588.779	109.813	−764.861	216.555		at 400 K
171	3-Ethyl-2,4--dimethylpentane	C	−56.18	112.30	−110.306	24.3612	−157.624	41.1531	0.07	0.129
		J	−235.06	469.86	−461.522	101.927	−659.499	172.185		at 298 K
172	2,2,3,3-Tetra-methylpentane	C	−56.70	106.69	−146.982	27.3214	−199.105	59.0020	0.08	0.251
		J	−237.23	446.39	−614.973	114.313	−833.054	246.864		at 400 K
173	2,2,3,4-Tetra-methylpentane	C	−56.64	108.23	−125.697	25.8011	−177.801	49.7683	0.06	0.150
		J	−236.98	452.83	−525.915	107.952	−743.921	208.230		at 298 K
174	2,2,4,4-Tetra-methylpentane	C	−57.83	103.13	−155.029	27.6267	−201.789	59.6852	0.09	0.282
		J	−241.96	431.50	−648.643	115.590	−844.286	249.723		at 400 K

Table I. (3. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
175	2,3,3,4-Tetra-methylpentane	C	−56.46	107.65	−126.402	25.8418	−178.496	50.1188	0.07	0.153
		J	−236.23	450.41	−528.867	108.122	−746.829	209.697	at 298 K	
176	Decane	C	−59.67	130.17	−22.1694	23.1021	−127.845	27.1954	0.10	0.331
		J	−249.66	544.63	−92.7568	96.6592	−534.902	113.786	at 400 K	
177	2-Methylnonane	C	−61.38	127.74	21.2178	21.9020	−114.783	21.9437	0.12	0.356
		J	−256.81	534.46	88.7752	91.6379	−480.253	91.8125	at 400 K	
178	3-Methylnonane	C	−60.70	129.12	−15.6834	23.1717	−129.635	27.7963	0.11	0.327
		J	−253.97	540.24	−65.6194	96.9504	−542.392	116.300	at 400 K	
179	4-Methylnonane	C	−60.70	129.12	−15.6834	23.1717	−129.635	27.7963	0.11	0.327
		J	−253.97	540.24	−65.6194	96.9504	−542.392	116.300	at 400 K	
180	5-Methylnonane	C	−60.70	127.74	−15.6834	23.1717	−129.635	27.7963	0.11	0.327
		J	−253.97	534.46	−65.6194	96.9504	−542.392	116.300	at 400 K	
181	3-Ethyloctane	C	−60.01	127.74	−52.5846	24.4414	−144.486	33.6489	0.10	0.298
		J	−251.08	534.46	−220.014	102.263	−604.531	140.787	at 400 K	
182	4-Ethyloctane	C	−60.01	129.12	−52.5846	24.4414	−144.486	33.6489	0.10	0.298
		J	−251.08	540.24	−220.014	102.263	−604.531	140.787	at 400 K	
183	2,2-Dimethyl-octane	C	−63.93	122.29	−31.7792	24.6524	−150.507	36.7619	0.13	0.398
		J	−267.48	511.66	−132.964	103.145	−629.721	153.812	at 400 K	
184	2,3-Dimethyl-octane	C	−62.41	126.01	−73.3785	25.2071	−153.139	36.8236	0.0.8	0.189
		J	−261.12	527.23	−307.016	105.466	−640.734	154.070	at 400 K	
185	2,4-Dimethyl-octane	C	−61.25	126.01	−38.2652	24.0373	−140.177	32.0096	0.09	0.227
		J	−256.27	527.23	−160.102	100.572	−586.499	133.928	at 400 K	
186	2,5-Dimethyl-octane	C	−62.41	126.01	−73.3785	25.2071	−153.139	36.8236	0.08	0.189
		J	−261.12	527.23	−307.016	105.466	−640.734	154,070	at 400 K	
187	2,6-Dimethyl-octane	C	−62.41	126.01	−73.3781	25.2070	−153.138	36.8235	0.08	0.189
		J	−261.12	527.23	−307.014	105.466	−640.731	154.069	at 400 K	
188	2,7-Dimethyl-octane	C	−63.10	123.25	−36.4773	23.9373	−138.287	30.9710	0.09	0.219
		J	−264.01	515.68	−152.621	100.154	−578.595	129.583	at 400 K	
189	3,3-Dimethyl-octane	C	−62.67	124.47	−68.6801	25.9220	−165.358	42.6144	0.12	0.370
		J	−262.21	520.78	−287.358	108.458	−691.858	178.298	at 400 K	
190	3,4-Dimethyl-octane	C	−60.56	126.70	−75.1664	25.3070	−155.028	37.8621	0.08	0.196
		J	−253.38	530.11	−314.496	105.885	−648.638	158.415	at 400 K	
191	3,5-Dimethyl-octane	C	−61.72	126.70	−110.280	26.4768	−167.991	42.6761	0.08	0.158
		J	−258.24	530.11	−461.410	110.779	−702.873	178.557	at 400 K	
192	3,6-Dimethyl-octane	C	−61.72	125.32	−110.280	26.4768	−167.991	42.6761	0.08	0.158
		J	−258.24	524.34	−461.410	110.779	−702.873	178.557	at 400 K	
193	4,4-Dimethyl-octane	C	−62.67	124.47	−68.6801	25.9220	−165.358	42.6144	0.12	0.370
		J	−262.21	520.78	−287.358	108.458	−691.858	178.298	at 400 K	
194	4,5-Dimethyl-octane	C	−60.56	125.32	−75.1664	25.3070	−155.028	37.8623	0.08	0.196
		J	−253.38	524.34	−314.496	105.885	−648.638	158.416	at 400 K	
195	4-Propylheptane	C	−60.01	125.56	−52.5844	24.4414	−144.486	33.6486	0.10	0.298
		J	−251.08	525.34	−220.013	102.263	−604.529	140.786	at 400 K	
196	4-Isopropyl-heptane	C	−60.02	124.63	−75.1661	25.3070	−155.028	37.8620	0.08	0.196
		J	−251.12	521.45	−314.495	105.884	−648.635	158.415	at 400 K	
197	3-Ethyl-2-methyl-heptane	C	− 60.56	126.01	−64.7389	24.7217	−145.648	33.2774	0.11	0.226
		J	−253.38	527.23	−270.868	103.435	−609.392	139.232	at 500 K	
198	4-Ethyl-2-methyl-heptane	C	−61.72	126.01	−71.6600	24.3089	−133.252	25.6957	0.24	0.745
		J	−258.24	527.23	−299.825	101.708	−557.525	107.511	at 500 K	
199	5-Ethyl-2-methyl-heptane	C	−61.72	124.63	−110.279	26.4767	−167.990	42.6760	0.08	0.158
		J	−258.24	521.45	−461.408	110.778	−702.870	178.556	at 400 K	

Table I. (4. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
200	3-Ethyl-3-methyl-heptane	C	−61.41	124.47	−105.582	27.1918	−180.210	48.4670	0.11	0.341
		J	−256.94	520.78	−441.754	113.771	−753.999	202.786		at 400 K
201	4-Ethyl-3-methyl-heptane	C	−59.87	126.70	−112.067	26.5767	−169.879	43.7146	0.08	0.166
		J	−250.50	530.11	−468.889	111.197	−710.774	182.902		at 400 K
202	3-Ethyl-5-methyl-heptane	C	−61.04	126.01	−147.180	27.7464	−182.841	48.5286	0.07	0.144
		J	−255.39	527.23	−615.802	116.091	−765.008	203.043		at 298 K
203	3-Ethyl-4-methyl-heptane	C	−59.87	126.01	−112.067	26.5767	−169.879	43.7146	0.08	0.166
		J	−250.50	527.23	−468.889	111.197	−710.774	182.902		at 400 K
204	4-Ethyl-4-methyl-heptane	C	−61.41	124.47	−105.581	27.1918	−180.209	48.4669	0.11	0.341
		J	−256.94	520.70	−441.752	113.770	−753.996	202.785		at 400 K
205	2,2,3-Trimethyl-heptane	C	−62.58	120.56	−91.2622	26.7877	−175.900	46.8279	0.09	0.271
		J	−261.83	504.42	−381.841	112.080	−735.967	195.928		at 400 K
206	2,2,4-Trimethyl-heptane	C	−63.06	120.56	−126.375	27.9574	−188.862	51.6417	0.08	0.234
		J	−263.84	504.42	−528.753	116.973	−790.198	216.069		at 400 K
207	2,2,5-Trimethyl-heptane	C	−64.95	120.56	−126.375	27.9574	−188.862	51.6417	0.08	0.234
		J	−271.75	504.42	−528.753	116.973	−790.198	216.069		at 400 K
208	2,2,6-Trimethyl-heptane	C	−65.64	119.18	−89.4739	26.6876	−174.011	45.7892	0.09	0.263
		J	−274.64	498.65	−374.359	111.661	−728.060	191.582		at 400 K
209	2,3,3-Trimethyl-heptane	C	−62.01	121.36	−91.2619	26.7876	−175.900	46.8277	0.09	0.271
		J	−259.45	507.77	−381.840	112.079	−735.964	195.927		at 400 K
210	2,3,4-Trimethyl-heptane	C	−61.11	123.59	−97.7479	26.1725	−165.569	42.0754	0.07	0.129
		J	−255.68	517.10	−408.977	109.506	−692.742	176.043		at 298 K
211	2,3,5-Trimethyl-heptane	C	−62.27	123.59	−132.861	27.3423	−178.532	46.8894	0.07	0.130
		J	−260.54	517.10	−555.890	114.400	−746.976	196.185		at 298 K
212	2,3,6-Trimethyl-heptane	C	−62.96	122.90	−95.9599	26.0726	−163.680	41.0369	0.07	0.127
		J	−263.42	514.21	−401.496	109.087	−684.838	171.698		at 298 K
213	2,4,4-Trimethyl-heptane	C	−62.49	121.36	−126.375	27.9574	−188.862	51.6417	0.08	0.234
		J	−261.46	507.77	−528.753	116.973	−790.198	216.069		at 400 K
214	2,4,5-Trimethyl-heptane	C	−62.27	123.59	−132.861	27.3423	−178.532	46.8894	0.07	0.130
		J	−260.54	517.10	−555.890	114.400	−746.976	196.185		at 298 K
215	2,4,6-Trimethyl-heptane	C	−60.52	121.52	−131.073	27.2423	−176.642	45.8509	0.06	0.128
		J	−253.22	508.44	−548.409	113.982	−739.072	191.840		at 298 K
216	2,5,5-Trimethyl-heptane	C	−64.38	121.36	−126.375	27.9574	−188.862	51.6417	0.08	0.234
		J	−269.37	507.77	−528.753	116.973	−790.198	216.069		at 400 K
217	3,3,4-Trimethyl-heptane	C	−61.32	122.74	−128.163	28.0573	−190.751	52.6803	0.08	0.241
		J	−256.56	513.54	−536.234	117.392	−798.103	220.414		at 400 K
218	3,3,5-Trimethyl-heptane	C	−61.80	122.74	−163.276	29.2271	−203.713	57.4943	0.08	0.204
		J	−258.57	513.54	−683.147	122.286	−852.337	240.556		at 400 K
219	3,4,4-Trimethyl-heptane	C	−61.32	122.74	−128.163	28.0573	−190.751	52.6803	0.08	0.241
		J	−256.56	513.54	−536.234	117.392	−798.103	220.414		at 400 K
220	3,4,5-Trimethyl-heptane	C	−60.43	123.59	−134.649	27.4423	−180.421	47.9280	0.07	0.132
		J	−252.84	517.10	−563.371	114.818	−754.881	200.530		at 298 K
221	3-Isopropyl-2-methylhexane	C	−61.11	121.52	−97.7479	26.1725	−165.569	42.0754	0.07	0.129
		J	−255.68	508.44	−408.977	109.506	−692.742	176.043		at 298 K
222	3,3-Diethylhexane	C	−60.15	122.29	−142.482	28.4651	−195.061	54.3194	0.10	0.312
		J	−251.67	511.66	−596.146	119.083	−816.135	227.272		at 400 K
223	3,4-Diethylhexane	C	−59.17	123.25	−148.969	27.8465	−184.731	49.5672	0.08	0.146
		J	−247.57	515.68	−623.286	116.510	−772.916	207.389		at 298 K
224	3-Ethyl-2,2-dimethylhexane	C	−61.83	120.56	−128.163	28.0573	−190.751	52.6803	0.08	0.241
		J	−258.95	504.42	−536.234	117.392	−798.103	220.414		at 400 K

Table I. (5. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
225	4-Ethyl-2,2-dimethylhexane	C	−62.37	119.18	−162.540	29.1814	−202.846	56.9831	0.07	0.200
		J	−260.96	498.65	−680.068	122.095	−848.708	238.417		at 400 K
226	3-Ethyl-2,3-dimethylhexane	C	−60.75	122.74	−128.163	28.0573	−190.751	52.6803	0.08	0.241
		J	−254.18	513.54	−536.234	117.392	−798.103	220.414		at 400 K
227	4-Ethyl-2,3-dimethylhexane	C	−60.43	122.90	−134.649	27.4423	−180.421	47.9280	0.07	0.132
		J	−252.84	514.21	−563.371	114.818	−754.881	200.530		at 298 K
228	3-Ethyl-2,4-dimethylhexane	C	−60.43	123.59	−134.649	27.4423	−180.421	47.9280	0.07	0.132
		J	−252.84	517.10	−563.371	114.818	−754.881	200.530		at 298 K
229	4-Ethyl-2,4-dimethylhexane	C	−61.23	121.36	−163.276	29.2271	−203.713	57.4943	0.08	0.204
		J	−256.19	507.77	−683.147	122.286	−852.337	240.556		at 400 K
230	3-Ethyl-2,5-dimethylhexane	C	−62.27	122.90	−132.861	27.3423	−178.532	46.8894	0.07	0.130
		J	−260.54	514.21	−555.890	114.400	−746.976	196.185		at 298 K
231	4-Ethyl-3,3-dimethylhexane	C	−60.63	121.36	−165.064	29.3270	−205.603	58.5328	0.08	0.211
		J	−253.68	507.77	−690.628	122.704	−860.241	244.901		at 400 K
232	3-Ethyl-3,4-dimethylhexane	C	−60.06	122.74	−165.064	29.3270	−205.603	58.5328	0.08	0.211
		J	−251.29	513.54	−690.628	122.704	−860.241	244.901		at 400 K
233	2,2,3,3-Tetramethylhexane	C	−61.63	115.91	−134.423	29.1327	−207.050	59.9242	0.09	0.279
		J	−257.86	484.97	−562.428	121.891	−866.295	250.723		at 400 K
234	2,2,3,4-Tetramethylhexane	C	−60.55	118.14	−150.745	28.9229	−201.293	56.8937	0.07	0.154
		J	−253.34	494.30	−630.716	121.013	−842.209	238.043		at 298 K
235	2,2,3,5-Tetramethylhexane	C	−64.29	117.45	−148.957	28.8229	−199.404	55.8551	0.07	0.152
		J	−268.99	491.41	−623.235	120.595	−834.305	233.698		at 298 K
236	2,2,4,4-Tetramethylhexane	C	−61.50	115.91	−179.372	30.7077	−224.586	66.4600	0.09	0.278
		J	−257.32	484.97	−750.495	128.481	−939.670	278.069		at 400 K
237	2,2,4,5-Tetramethylhexane	C	−63.61	117.45	−148.957	28.8229	−199.404	55.8551	0.07	0.152
		J	−266.14	491.41	−623.237	120.595	−834.309	233.699		at 298 K
238	2,2,5,5-Tetramethylhexane	C	−68.18	112.35	−142.471	29.4381	−209.735	60.6079	0.09	0.307
		J	−285.27	470.07	−596.100	123.169	−877.531	253.582		at 400 K
239	2,3,3,4-Tetramethylhexane	C	−60.66	119.63	−150.745	28.9230	−201.294	56.8941	0.07	0.154
		J	−253.80	500.53	−630.718	121.014	−842.213	238.044		at 298 K
240	2,3,3,5-Tetramethylhexane	C	−61.83	118.25	−148.957	28.8230	−199.405	55.8555	0.07	0.151
		J	−258.70	494.76	−623.237	120.595	−834.309	233.699		at 298 K
241	2,3,4,4-Tetramethylhexane	C	−59.98	119.63	−150.745	28.9230	−201.294	56.8941	0.07	0.154
		J	−250.96	500.53	−630.718	121.014	−842.213	238.044		at 298 K
242	2,3,4,5-Tetramethylhexane	C	−61.67	119.10	−120.330	27.0382	−176.112	46.2892	0.06	0.118
		J	−258.03	498.31	−503.461	113.128	−736.151	193.673		at 298 K
243	3,3,4,4-Tetramethylhexane	C	−60.37	116.71	−171.325	30.4026	−221.902	65.7772	0.08	0.250
		J	−252.59	488.31	−716.825	127.204	−928.438	275.211		at 400 K
244	2,4-Dimethyl-3-isopropylpentane	C	−61.67	116.23	−150.745	28.9230	−201.294	56.8941	0.07	0.154
		J	−258.03	486.31	−630.718	121.014	−842.213	238.044		at 298 K
245	3,3-Diethyl-2-methylpentane	C	−59.49	119.18	−165.065	29.3271	−205.604	58.5332	0.08	0.212
		J	−248.91	498.65	−690.631	122.705	−860.245	244.902		at 400 K
246	3-Ethyl-2,2,3-trimethylpentane	C	−60.37	117.29	−171.325	30.4026	−221.902	65.7772	0.08	0.250
		J	−252.59	490.74	−716.825	127.204	−928.438	275.211		at 400 K
247	3-Ethyl-2,2,4-trimethylpentane	C	−60.55	115.91	−150.745	28.9230	−201.294	56.8938	0.07	0.154
		J	−253.34	484.97	−630.718	121.014	−842.213	238.044		at 298 K
248	3-Ethyl-2,3,4-trimethylpentane	C	−60.09	118.25	−148.783	28.8012	−198.981	55.5308	0.06	0.149
		J	−251.42	494.76	−622.509	120.504	−832.536	232.341		at 298 K
249	2,2,3,3,4-Pentamethylpentane	C	−59.08	112.80	−137.335	29.1879	−208.445	60.6943	0.06	0.138
		J	−247.19	471.96	−574.611	122.122	−872.133	253,945		at 298 K

Table I. (6. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
250	2,2,3,4,4-Penta-methylpentane	C	−59.04	110.62	−166.841	30.4036	−222.166	65.8599	0.08	0.216
		J	−247.02	462.83	−698.063	127.209	−929.542	275.556		at 400 K
251	Undecane	C	−64.60	139.48	−26.8042	25.5186	−143.578	31.6159	0.10	0.338
		J	−270.29	583.58	−112.149	106.770	−600.731	132.280		at 400 K
252	Dodecane	C	−69.52	148.78	−29.0415	27.7842	−156.370	34.2766	0.10	0.325
		J	−290.87	622.50	−121.510	116.249	−654.255	143.413		at 400 K
253	Tridecane	C	−74.45	158.09	−31.3571	30.0557	−169.314	37.0385	0.10	0.322
		J	−311.50	661.45	−131.198	125.753	−708.408	154.969		at 400 K
254	Tetradecane	C	−79.38	167.40	−35.6392	32.4494	−184.606	41.2082	0.10	0.326
		J	−332.13	700.40	−149.114	135.768	−772.392	172.415		at 400 K
255	Pentadecane	C	−84.31	176.71	−38.0935	34.7260	−197.572	43.9535	0.10	0.326
		J	−352.75	739.35	−159.383	145.293	−826.639	183.900		at 400 K
256	Hexadecane	C	−89.23	186.02	−39.9948	36.9731	−210.101	46.4996	0.10	0.320
		J	−373.34	778.31	−167.338	154,695	−879.063	194.554		at 400 K
257	Heptadecane	C	−94.15	195.33	−44.6911	39.3911	−225.808	50.8851	0.10	0.327
		J	−393.92	817.26	−186.988	164.812	−944.778	212.903		at 400 K
258	Octadecane	C	−99.08	204.64	−46.6541	41.6399	−238.310	53.3966	0.10	0.324
		J	−414.55	856.21	−195.201	174.221	−997.088	223.411		at 400 K
259	Nonadecane	C	−104.00	213.95	−48.8362	43.9042	−251.152	56.1132	0.10	0.320
		J	−435.14	895.17	−204.331	183.695	−1050.82	234.777		at 400 K
260	Eicosane	C	−108.93	223.26	−53.4624	46.3158	−266.696	60.3917	0.10	0.326
		J	−455.76	934.12	−223.687	193.785	−1115.86	252.679		at 400 K
261	Ethylene	C	12.50	52.45	9.09005	3.73965	−19.9360	4.19088	0.11	0.356
		J	52.30	219.45	38.0327	15.6467	−83.4124	17.5346		at 400 K
262	Propene	C	4.88	63.80	12.1642	5.39215	−23.8708	3.17470	0.11	0.360
		J	20.42	266.94	50.8950	22.5607	−99.8733	13.2829		at 400 K
263	1-Butene	C	−0.03	73.04	−9.58677	8.54739	−49.1797	11.4753	0.06	0.217
		J	−0.13	305.60	−40.1110	35.7622	−205.768	48.0124		at 400 K
264	2-Butene, cis	C	−1.67	71.90	−12.4250	7.69408	−33.3051	3.72688	0.15	0.464
		J	−6.99	300.83	−51.9863	32.1920	−139.348	15.5933		at 400 K
265	2-Butene, trans	C	−2.67	70.86	28.4367	6.87311	−27.3093	2.28571	0.11	0.356
		J	−11.17	293.59	118.979	28.7570	−114.262	9.56338		at 400 K
266	2-Methylpropene	C	−4.04	70.17	15.0138	7.78551	−41.0994	8.58453	0.05	0.176
		J	−16.90	293.59	62.8179	32.5746	−171.960	35.9177		at 400 K
267	1-Pentene	C	−5.00	82.65	9.37615	9.89924	−49.0280	8.28006	0.23	0.713
		J	−20.92	345.81	39.2297	41.4183	−205.133	34.6437		at 298 K
268	2-Pentene, cis	C	−6.71	82.76	−37.2040	11.1466	−62.8738	13.8833	0.12	0.393
		J	−28.07	346.27	−155.661	46.6372	−263.064	58.0874		at 400 K
269	2-Pentene, trans	C	−7.59	81.36	5.39978	9.92839	−50.5928	9.55564	0.09	0.306
		J	−31.76	340.41	22.5927	41.5404	−211.680	39.9808		at 400 K
270	2-Methyl-1-butene	C	−8.68	81.15	−0.67429	10.3890	−55.6257	11.2103	0.10	0.318
		J	−36.32	339.53	−2.82125	43.4676	−232.738	46.9037		at 400 K
271	3-Methyl-1-butene	C	−6.92	79.70	15.3871	10.9250	−70.5366	19.5920	0.05	0.151
		J	−28.95	333.46	64.3793	45.7103	−295.126	81.9730		at 400 K
272	2-Methyl-2-butene	C	−10.17	80.92	−3.15847	9.89337	−48.7067	8.60660	0.08	0.269
		J	−42.55	338.57	−13.2151	41.3939	−203.789	36.0519		at 400 K
273	1-Hexene	C	−9.96	91.93	−4.17211	12.6789	−69.3163	14.4616	0.08	0.333
		J	−41.67	384.64	−17.4562	53.0483	−290.020	60.5073		at 400 K
274	2-Hexene, cis	C	−12.51	92.37	−29.8244	13.0524	−71.1780	14.8058	0.14	0.481
		J	−52.34	386.48	−124.786	54.6115	−297.810	61.9475		at 400 K

Table I. (7. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
275	2-Hexene, trans	C	−12.88	90.97	12.5935	11.8369	−58.7363	10.2574	0.13	0.415
		J	−53.89	380.62	52.6912	49.5255	−245.752	42.9169		at 400 K
276	3-Hexene, cis	C	−11.38	90.73	−58.2666	14.2453	−86.5308	21.0675	0.13	0.408
		J	−47.61	379.61	−243.787	59.6022	−362.045	88.1462		at 400 K
277	3-Hexene, trans	C	−13.01	89.59	−13.3671	13.3325	−81.4189	20.7995	0.09	0.242
		J	−54.43	374.84	−55.9278	55.7832	−340.657	87.0251		at 400 K
278	2-Methyl-1-pentene	C	−12.49	91.34	4.47136	12.7050	−71.3569	15.6520	0.04	0.126
		J	−52.26	382.17	18.7082	53.1575	−298.557	65.4879		at 400 K
279	3-Methyl-1-pentene	C	−10.76	90.06	7.87744	13.5864	−88.8683	24.5363	0.05	0.104
		J	−45.02	376.81	32.9591	56.8456	−371.826	102.660		at 700 K
280	4-Methyl-1-pentene	C	−10.54	87.89	−31.5229	13.3763	−78.5756	18.6291	0.07	0.187
		J	−44.10	367.73	−131.893	55.9664	−328.761	77.9442		at 400 K
281	2-Methyl-2-pentene	C	−14.28	90.45	−38.4962	13.7258	−83.0584	20.7328	0.08	0.233
		J	−59.75	378.44	−161.069	57.4289	−347.518	86.7462		at 400 K
282	3-Methyl-2-pentene, cis	C	−13.80	90.45	−38.4962	13.7258	−83.0584	20.7328	0.08	0.233
		J	−57.74	378.44	−161.069	57.4289	−347.518	86.7462		at 400 K
283	3-Methyl-2-pentene, trans	C	−14.02	91.26	−38.4962	13.7258	−83.0584	20.7328	0.08	0.233
		J	−58.66	381.83	−161.069	57.4289	−347.518	86.7462		at 400 K
284	4-Methyl-2-pentene, cis	C	−12.03	89.23	−4.00491	12.8434	−72.7146	16.1337	0.22	0.802
		J	−50.33	373.34	−16.7566	53.7369	−304.238	67.5034		at 400 K
285	4-Methyl-2-pentene, trans	C	−12.99	88.02	30.1614	12.3110	−71.8228	17.4999	0.02	0.051
		J	−54.35	368.28	126.195	51.5091	−300.508	73.2199		at 300 K
286	2-Ethyl-1-butene	C	−12.32	90.01	−31.7052	14.3860	−95.9739	27.1871	0.05	0.141
		J	−51.55	376.60	−132.655	60.1911	−401.556	113.751		at 400 K
287	2,3-Dimethyl-1-butene	C	−13.32	87.39	19.6228	13.1893	−85.7122	24.0734	0.06	0.127
		J	−55.73	365.64	82.1017	55.1839	−358.621	100.723		at 400 K
288	3,3-Dimethyl-1-butene	C	−10.31	82.16	−40.1920	13.6833	−79.5127	17.5833	0.21	0.555
		J	−43.14	343.76	−168.164	57.2508	−332.683	73.5688		at 400 K
289	2,3-Dimethyl-2-butene	C	−14.15	87.15	16.5298	10.2879	−31.1702	2.27860	0.16	0.141
		J	−59.20	364.64	69.1606	43.0447	−130.416	−9.53369		at 400 K
290	1-Heptene	C	−14.89	101.24	−7.88735	15.0360	−83.8660	18.1656	0.09	0.274
		J	−62.30	423.59	−33.0008	62.9107	−350.896	76.0050		at 400 K
291	1-Octene	C	−19.82	110.55	−9.78879	17.2832	−96.3957	20.7119	0.08	0.270
		J	−82.93	462.54	−40.9565	72.3128	−403.320	86.6587		at 400 K
292	1-Nonene	C	−24.74	119.86	−11.9623	19.5427	−109.048	23.2867	0.08	0.274
		J	−103.51	501.49	−50.0506	81.7665	−456.260	97.4315		at 400 K
293	1-Decene	C	−29.67	129.17	−16.5971	21.9591	−124.782	27.7077	0.09	0.287
		J	−124.14	540.45	−69.4423	91.8768	−522.087	115.926		at 400 K
294	1-Undecene	C	−34.60	138.48	−19.1151	24.2419	−137.887	30.5380	0.08	0.278
		J	−144.77	579.40	−79.9776	101.428	−576.920	127.771		at 400 K
295	1-Dodecene	C	−39.52	147.78	−21.0781	26.4906	−150.390	33.0495	0.08	0.278
		J	−165.35	618.31	−88.1906	110.837	−629.230	138.279		at 400 K
296	1-Tridecene	C	−44.45	157.09	−22.9795	28.7378	−162.919	35.5957	0.08	0.275
		J	−185.98	657.26	−96.1462	120.239	−681.653	148.932		at 400 K
297	1-Tetradecene	C	−49.36	166.40	−27.8864	31.1666	−178.776	40.0446	0.09	0.288
		J	−206.52	696.22	−116.677	130.401	−747.998	167.546		at 400 K
298	1-Pentadecene	C	−54.31	175.71	−30.0686	33.4309	−191.619	42.7612	0.09	0.286
		J	−227.23	735.17	−125.807	139.875	−801.732	178.913		at 400 K
299	1-Hexadecene	C	−59.23	185.02	−32.0315	35.6796	−204.021	45.2726	0.08	0.300
		J	−247.82	774.12	−134.020	149.283	−854.040	189.420		at 400 K

Table I. (8. cont.)

No.	Compound		$H\dot{a}_f^\circ$ 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
300	1-Heptadecene	C	−64.15	194.33	−36.4471	38.0805	−219.514	49.4879	0.08	0.294
		J	−268.40	813.08	−152.495	159.329	−918.448	207.057	at 400 K	
301	1-Octadecene	C	−69.08	203.64	−38.6292	40.3447	−232.356	52.2045	0.09	0.291
		J	−289.03	852.03	−61.625	168.802	−972.179	218.423	at 400 K	
302	1-Nonadecene	C	−74.00	212.95	−41.0836	42.6214	−245.323	54.9496	0.09	0.293
		J	−309.62	890.98	−171.894	178.328	−1026.43	229.909	at 400 K	
303	1-Eicosene	C	−78.93	222.26	−45.4377	45.0208	−260.743	59.1997	0.09	0.297
		J	−330.24	929.94	−190.111	188.367	−1090.95	247.692	at 400 K	
304	Allene	C	45.92	58.30	15.7092	5.17981	−35.9228	10.5582	0.03	0.055
		J	192.13	243.93	65.7272	21.6723	−150.301	44.1754	at 500 K	
305	1,2-Butadiene	C	38.77	70.03	23.4488	6.69210	−38.1442	8.89410	0.05	0.167
		J	162.21	293.01	98.1095	27.9997	−159.595	37.2128	at 400 K	
306	1,3-Butadiene	C	26.33	66.62	−38.9642	9.88036	−81.8327	27.4669	0.06	0.138
		J	110.16	278.74	−163.026	41.3394	−342.388	114.922	at 500 K	
307	1,2-Pentadiene	C	34.80	79.70	5.95325	10.1418	−69.3111	20.1094	0.06	0.128
		J	145.60	333.46	24.9084	42.4333	−289.997	84.1373	at 400 K	
308	1,3-Pentadiene, cis	C	18.70	77.50	−64.1532	12.2066	−91.6435	28.2011	0.09	0.193
		J	78.24	324.26	−268.417	51.0725	−383.437	117.993	at 500 K	
309	1,3-Pentadiene, trans	C	18.60	76.40	−19.6331	11.1821	−82.0453	24.7939	0.08	0.177
		J	77.82	319.66	−82.1448	46.7860	−343.277	103.277	at 500 K	
310	1,4-Pentadiene	C	25.20	73.70	−1.01453	10.4662	−74.2881	22.4402	0.06	0.130
		J	105.44	333.46	−4.2448	43.7905	−310.821	93.8898	at 700 K	
311	2,3-Pentadiene	C	33.10	77.60	29.8861	8.28752	−41.8414	7.97643	0.06	0.182
		J	138.49	324.68	125.043	34.6749	−175.065	33.3733	at 400 K	
312	3-Methyl-1,2-butadiene	C	31.00	76.40	29.5424	8.91161	−52.5366	12.8699	0.03	0.060
		J	129.70	319.66	123.605	37.2862	−219.813	53.8477	at 400 K	
313	2-Methyl-1,3-butadiene	C	18.10	75.44	−36.0800	12.2833	−99.4281	33.1289	0.09	0.173
		J	75.73	315.64	−150.959	51.3932	−416.007	138.611	at 298 K	
314	Acetylene	C	54.19	48.00	37.8032	3.06220	−30.5447	12.0855	0.19	0.458
		J	226.73	200.83	158.169	12.8122	−127.799	50.5659	at 400 K	
315	Propyne	C	44.32	59.30	35.1251	4.45231	−28.0207	7.69991	0.03	0.044
		J	185.43	248.11	146.963	18.6284	−117.239	32.2164	at 500 K	
316	Butadiyne	C	113.00	59.76	58.2603	5.38236	−54.0162	21.0166	0.21	0.559
		J	472.79	250.04	243.761	22.5198	−226.004	87.9334	at 400 K	
317	1-Buten-3-yne	C	72.80	66.77	16.1386	6.78355	−54.0850	17.8117	0.07	0.120
		J	304.60	279.37	67.5238	28.3824	−226.292	74.5240	at 400 K	
318	1-Butyne	C	39.48	69.51	21.9537	7.01411	−44.6876	12.1932	0.03	0.051
		J	165.18	290.83	91.8541	29.3470	−186.973	51.0162	at 400 K	
319	2-Butyne	C	34.97	67.71	45.2148	5.26277	−18.0461	0.16668	0.11	0.334
		J	146.31	283.30	189.179	22.0194	−75.5049	0.69738	at 400 K	
320	1-Pentyne	C	34.56	78.82	38.6149	8.62586	−49.2686	11.3206	0.11	0.341
		J	144.35	329.78	161.565	36.0906	−206.140	47.3652	at 400 K	
321	2-Pentyne	C	30.80	79.30	29.1619	7.99315	−37.4954	6.04213	0.09	0.260
		J	128.87	331.79	122.013	33.4433	−156.881	25.2803	at 400 K	
322	3-Methyl-1-butyne	C	32.60	76.23	11.1498	9.74372	−62.8681	16.7256	0.04	0.119
		J	136.40	318.95	46.6506	40.7677	−263.040	69.9798	at 700 K	
323	1-Hexyne	C	29.55	88.13	28.2428	11.1164	−64.5223	15.0847	0.05	0.163
		J	123.64	368.74	118.168	46.5111	−269.961	63.1145	at 400 K	
324	1-Heptyne	C	24.62	97.44	25.3603	13.4245	−78.2087	18.3126	0.05	0.184
		J	103.01	407.69	106.107	56.1681	−327.225	76.6199	at 400 K	

Table I. (9. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
325	1-Octyne	C	19.70	106.75	23.1867	15.6840	−90.8615	20.8874	0.06	0.200
		J	82.42	446.64	97.0132	65.6218	−380.165	87.3927		at 400 K
326	1-Nonyne	C	14.77	116.06	18.5519	18.1004	−106.595	25.3077	0.07	0.223
		J	61.80	485.60	77.6212	75.7323	−445.993	105.888		at 400 K
327	1-Decyne	C	9.85	125.36	16.0339	20.3832	−119.700	28.1387	0.07	0.221
		J	41.21	524.51	67.0859	85.2834	−500.826	117.732		at 400 K
328	1-Undecyne	C	4.92	134.67	14.0709	22.6320	−132.203	30.6502	0.07	0.226
		J	20.59	563.46	58.8728	94.6921	−553.136	128.240		at 400 K
329	1-Dodecyne	C	−0.01	143.98	9.71681	25.0313	−147.624	34.9002	0.07	0.239
		J	0.04	602.41	40.6551	104.731	−617.657	146.023		at 400 K
330	1-Tridecyne	C	−4.93	153.29	8.48471	27.2532	−159.810	37.2898	0.07	0.252
		J	−20.63	641.37	35.5000	114.027	−668.644	156.021		at 400 K
331	1-Tetradecyne	C	−9.86	162.60	5.08047	29.5722	−173.431	40.3619	0.07	0.247
		J	−41.25	680.32	21.2567	123.730	−725.637	168.874		at 400 K
332	1-Pentadecyne	C	−14.78	171.91	0.66481	31.9731	−188.825	44.5772	0.08	0.258
		J	−61.84	719.27	2.78156	133.775	−790.044	186.511		at 400 K
333	1-Hexadecyne	C	−19.71	181.22	−1.29817	34.2218	−201.328	47.0886	0.08	0.259
		J	−82.47	758.22	−5.43154	143.184	−842.355	197.019		at 400 K
334	1-Heptadecyne	C	−24.64	190.53	−3.48028	36.4861	−214.170	49.8052	0.08	0.259
		J	−103.09	797.18	−14.5615	152.658	−896.087	208.385		at 400 K
335	1-Octadecyne	C	29.56	199.84	−8.38719	38.9149	−230.027	54.2541	0.08	0.271
		J	−123.68	836.13	−35.0920	162.820	−962.431	226.999		at 400 K
336	1-Nonadecyne	C	−34.49	209.15	−10.2886	41.1621	−242.556	56.8004	0.08	0.269
		J	−144.31	875.08	−43.0476	172.222	−1014.86	237.653		at 400 K
337	1-Eicosyne	C	−39.41	218.46	−12.2516	43.4108	−255.059	59.3119	0.08	0.269
		J	−164.89	914.04	−51.2607	181.631	−1067.17	248.161		at 400 K
338	Cyclopropene	C	12.74	56.75	−72.3129	8.53656	−60.0680	17.3163	0.16	0.556
		J	53.30	237.44	−302.557	35.7170	−251.324	72.4514		at 400 K
339	Cyclobutane	C	6.37	63.43	−90.4082	10.5769	−63.6895	14.9042	0.16	0.584
		J	26.65	265.39	−378.268	44.2537	−266.477	62.3594		at 400 K
340	Cyclopentane	C	−18.46	70.00	−133.049	13.1352	−72.3998	14.1392	0.21	0.620
		J	−77.24	292.88	−556.676	54.9577	−302.921	59.1582		at 400 K
341	Cyclohexane	C	−29.43	71.28	−132.165	14.7597	−62.4665	3.80884	0.22	0.697
		J	−123.14	298.24	−552.976	61.7546	−261.360	15.9362		at 400 K
342	Cycloheptane	C	−28.52	81.82	−181.970	18.7875	−100.394	18.0576	0.17	0.537
		J	−119.33	342.33	−761.361	78.6068	−420.050	75.5530		at 400 K
343	Cyclooctane	C	−30.06	87.66	−231.792	22.8188	−138.446	32.4059	0.12	0.414
		J	−125.77	366.77	−969.817	95.4737	−579.257	135.586		at 400 K
344	Cyclobutene	C	31.00	62.98	−66.1323	9.31935	−63.0929	17.0345	0.09	0.321
		J	129.70	263.51	−276.697	38.9922	−263.981	71.2722		at 400 K
345	Cyclopentene	C	7.87	69.23	−93.1607	10.6645	−53.9373	8.50310	0.21	0.698
		J	32.93	289.66	−389.784	44.6203	−225.674	35.5769		at 400 K
346	Cyclohexene	C	−1.28	74.27	−140.313	16.1870	−112.148	30.9151	0.09	0.322
		J	−5.36	310.75	−587.071	67.7265	−469.225	129.349		at 400 K
347	Methylcyclo-pentane	C	−25.50	81.24	−121.012	15.2734	−86.7055	18.4687	0.16	0.528
		J	−106.69	339.91	−506.313	63.9038	−362.776	77.2731		at 400 K
348	Ethylcyclo-pentane	C	−30.37	90.42	−151.133	19.1145	−126.155	35.3326	0.29	0.575
		J	−127.07	378.32	−632.342	79.9750	−527.833	147.831		at 500 K
349	1,1-Dimethyl-cyclopentane	C	−33.05	85.87	−140.026	18.3665	−107.169	23.2781	0.18	0.585
		J	−138.28	359.38	−585.870	76.8453	−448.395	97.3955		at 400 K

Table I. (10 cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
350	1,2-Dimethyl-cyclopentane, cis	C	−30.96	87.51	−136.896	18.3715	−109.072	24.5622	0.17	0.562
		J	−129.54	366.14	−572.772	76.8665	−456.358	102.768		at 400 K
351	1,2-Dimethyl-cyclopentane, trans	C	−32.67	87.67	−135.635	18.3870	−110.249	25.3078	0.18	0.579
		J	−136.69	366.81	−567.496	76.9313	−461.280	105.888		at 400 K
352	1,3-Dimethyl-cyclopentane, cis	C	−32.47	87.67	−135.635	18.3870	−110.249	25.3078	0.18	0.579
		J	−135.85	366.81	−567.496	76.9313	−461.280	105.888		at 400 K
353	1,3-Dimethyl-cyclopentane, trans	C	−31.93	87.67	−135.635	18.3870	−110.249	25.3078	0.18	0.579
		J	−133.60	366.81	−567.496	76.9313	−461.280	105.888		at 400 K
354	Propylcyclo-pentane	C	−35.39	99.73	−154.357	21.4411	−140.126	38.6958	0.24	0.875
		J	−148.07	417.27	−645.831	89.7097	−586.288	161.903		at 400 K
355	Butylcyclopentane	C	−40.22	109.04	−278.892	31.2972	−297.213	126.432	0.47	0.824
		J	−168.28	456.22	−1166.89	130.947	−1243.54	528.990		at 500 K
356	1-Cyclopentyl-pentane	C	−45.15	118.35	−160.885	26.1000	−168.100	45.5206	0.16	0.589
		J	−188.91	495.18	−673.143	109.202	−703.747	190.458		at 400 K
357	1-Cyclopentyl-hexane	C	−50.07	127.66	−163.068	28.3643	−181.043	48.2373	0.14	0.532
		J	−209.49	534.13	−682.276	118.676	−757.483	201.825		at 400 K
358	1-Cyclopentyl-heptane	C	−55.00	136.96	−165.586	30.6471	−194.148	51.0682	0.12	0.467
		J	−230.12	573.04	−692.811	128.227	−812.316	213.669		at 400 K
359	1-Cyclopentyl-octane	C	−59.92	146.27	−142.566	31.3539	−180.526	40.3667	0.12	0.796
		J	−250.71	611.99	−596.498	131.185	−755.321	168.894		at 400 K
360	1-Cyclopentyl-nonane	C	−64.85	155.58	−171.903	35.2952	−222.071	57.8298	0.09	0.347
		J	−271.33	650.95	−719.242	147.675	−929.146	241.960		at 400 K
361	1-Cyclopentyl-decane	C	−69.78	164.89	−174.357	37.5718	−235.037	60.5749	0.08	0.300
		J	−291.96	689.90	−729.510	157.200	−983.394	253.445		at 400 K
362	1-Cyclopentyl-undecane	C	−74.70	174.20	−178.992	39.9882	−250.770	64.9952	0.07	0.254
		J	−312.54	728.85	−748.902	167.311	−1049.22	271.940		at 400 K
363	1-Cyclopentyl-dodecane	C	−80.28	183.51	−180.955	42.2370	−263.273	67.5067	0.06	0.222
		J	−335.89	767.81	−757.115	176.720	−1101.53	282.448		at 400 K
364	1-Cyclopentyl-tridecane	C	−84.55	192.89	−182.918	44.4857	−275.775	70.0182	0.05	0.190
		J	−353.76	807.05	−765.328	186.128	−1153.84	292.956		at 400 K
365	1-Cyclopentyl-tetradecane	C	−89.48	202.13	−187.553	46.9022	−291.509	74.4386	0.05	0.161
		J	−374.38	845.71	−784.720	196.239	−1219.67	311.451		at 400 K
366	1-Cyclopentyl-pentadecane	C	−94.41	211.44	−190.007	49.1788	−304.474	77.1836	0.04	0.136
		J	−395.01	884.66	−794.989	205.764	−1273.92	322.936		at 400 K
367	1-Cyclopentylhexa-decane	C	−99.33	220.75	−191.908	51.4259	−317.004	79.7299	0.04	0.117
		J	−415.60	923.62	−802.944	215.166	−1326.34	333.590		at 400 K
368	1-Methylcyclo-pentene	C	−1.30	78.00	−70.4254	11.8711	−48.6942	1.14169	0.49	0.684
		J	−5.44	326.35	−294.660	49.6686	−203.736	4.77683		at 400 K
369	3-Methylcyclo-pentene	C	2.07	79.00	−103.268	13.6111	−78.4507	16.6087	0.21	0.087
		J	8.66	330.54	−432.073	57.1582	−328.238	69.4907		at 400 K
370	4-Methylcyclo-pentene	C	3.53	78.60	−98.3732	13.4115	−74.9855	15.0786	0.16	0.537
		J	14.77	328.86	−411.594	56.1137	−313.739	63.0887		at 400 K
371	Methylcyclohexane	C	−36.99	82.06	−138.731	18.1448	−94.6485	15.8052	0.16	0.502
		J	−154.77	343.34	−580.450	75.9177	−396.009	66.1289		at 400 K
372	Ethylcyclohexane	C	−41.05	91.44	−143.558	20.6637	−110.873	19.8402	0.13	0.442
		J	−171.75	382.58	−600.648	86.4571	−463.892	83.0112		at 400 K
373	1,1-Dimethyl-cyclohexane	C	−43.26	87.24	−148.827	20.048	−93.357	9.86533	0.19	0.601
		J	−181.00	365.01	−622.691	83.8838	−390.608	41.2765		at 400 K
374	1,2-Dimethylcyclo-hexane, cis	C	−41.15	89.51	−150.540	20.6199	−107.111	17.3019	0.18	0.574
		J	−172.17	374.51	−629.859	86.2735	−448.153	72.3913		at 400 K

Table I. (11. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
375	1,2-Dimethylcyclo-	C	−43.02	88.65	−159.917	21.5245	−122.195	24.5849	0.14	0.439
	hexane, trans	J	−180.00	370.91	−669.095	90.0586	−511.262	102.863	at 400 K	
376	1,3-Dimethylcyclo-	C	−44.16	88.54	−140.710	20.1726	−100.137	14.3830	0.20	0.618
	hexane, cis	J	−184.77	370.45	−588.73	84.4023	−418.973	60.1784	at 400 K	
377	1,3-Dimethylcyclo-	C	−42.20	89.92	−139.711	20.2181	−103.205	16.0051	0.18	0.608
	hexane, trans	J	−176.56	376.23	−584.550	84.5925	−431.811	66.9652	at 400 K	
378	1,4-Dimethylcyclo-	C	−42.22	88.54	−142.518	20.3892	−106.333	17.7079	0.19	0.632
	hexane, cis	J	−176.65	370.45	−596.294	85.3083	−444.895	74.0900	at 400 K	
379	1,4-Dimethylcyclo-	C	−44.12	87.19	−160.219	21.2938	−116.714	21.6413	0.16	0.509
	hexane, trans	J	−184.60	364.80	−670.357	89.0933	−488.333	90.5472	at 400 K	
380	Propylcyclo-	C	−46.20	100.27	−148.184	23.4670	−133.789	27.2734	0.14	0.486
	hexane	J	−193.30	419.53	−620.001	98.1859	−559.772	114.112	at 400 K	
381	1,3,5-Trimethylcyc-	C	−51.48	93.30	−142.688	22.2005	−105.625	12.9607	0.23	0.706
	lohexane, cis, cis	J	−215.39	390.37	−597.007	92.8867	−441.934	54.2278	at 400 K	
382	1,3,5-Trimethylcyc-	C	−49.37	95.60	−146.304	22.6335	−118.016	19.6106	0.22	0.731
	lohexane, cis, trans	J	−206.56	400.00	−612.134	94.6986	−493.780	82.0509	at 400 K	
383	Butylcyclohexane	C	−50.95	109.58	−144.115	25.3661	−140.441	26.8306	0.13	0.452
		J	−213.17	458.48	−602.975	106.102	−587.605	112.259	at 400 K	
384	Pentylcyclohexane	C	−55.88	118.89	−156.385	28.2191	−163.322	34.7931	0.14	0.454
		J	−233.80	497.44	−654.315	118.069	−683.338	145.574	at 400 K	
385	1-Cyclohexyl-	C	−60.80	128.20	−159.248	30.5267	−177.040	38.0185	0.14	0.484
	hexane	J	−254.39	536.39	−666.294	127.724	−740.735	159.069	at 400 K	
386	1-Cyclohexyl-	C	−65.73	137.51	−162.853	32.8748	−191.239	41.4107	0.12	0.420
	heptane	J	−275.01	575.34	−681.375	137.548	−800.145	173.262	at 400 K	
387	1-Cyclohexyl-	C	−70.65	146.82	−158.783	34.7740	−197.891	40.9679	0.12	0.400
	octane	J	−295.60	614.29	−664.349	145.494	−827.977	171.410	at 400 K	
388	1-Cyclohexyl-	C	−75.58	156.12	−163.380	37.1779	−213.225	45.0955	0.13	0.439
	nonane	J	−316.23	653.21	−683.582	155.552	−892.134	188.680	at 400 K	
389	1-Cyclohexyl-	C	−80.51	165.43	−173.198	39.8787	−233.215	51.3542	0.13	0.432
	decane	J	−336.85	692.16	−724.660	166.853	−975.771	214.866	at 400 K	
390	1-Cyclohexyl-	C	−85.43	174.74	−169.848	41.8336	−241.143	51.7131	0.12	0.414
	undecane	J	−357.44	731.11	−710.643	175.032	−1008.94	216.368	at 400 K	
391	1-Cyclohexyl-	C	−90.36	184.05	−175.905	44.3340	−258.233	56.8091	0.11	0.380
	dodecane	J	−378.07	770.07	−735.985	185.493	−1080.45	237.689	at 400 K	
392	1-Cyclohexyl-	C	−95.28	193.36	−178.049	46.5857	−270.676	59.2328	0.12	0.404
	tridecane	J	−398.65	809.02	−744.956	194.915	−1132.51	247.830	at 400 K	
393	1-Cyclohexyltetra-	C	−100.21	202.67	−180.193	48.8375	−283.118	61.6566	0.12	0.425
	decane	J	−419.28	847.97	−753.927	204.336	−1184.57	257.971	at 400 K	
394	1-Cyclohexylpenta-	C	−105.14	211.98	−186.250	51.3378	−300.208	66.7526	0.12	0.395
	decane	J	−439.91	886.92	−779.270	214.798	−1256.07	279.293	at 400 K	
395	1-Cyclohexyl-	C	−110.06	221.29	−182.900	53.2928	−308.106	67.1115	0.11	0.383
	hexadecane	J	−460.49	925.88	−765.253	222.976	−1289.24	280.794	at 400 K	
396	Benzene	C	19.82	64.34	−104.593	12.5040	−89.8842	25.4575	0.07	0.241
		J	82.93	269.20	−437.617	52.3169	−376.076	106.514	at 400 K	
397	Toluene	C	11.95	76.64	−104.292	14.4239	−95.4442	24.9345	0.10	0.331
		J	50.00	320.66	−436.357	60.3494	−399.338	104.326	at 400 K	
398	Ethylbenzene	C	7.12	86.15	−102.917	16.8889	−114.909	31.0676	0.07	0.261
		J	29.79	360.45	−430.603	70.6631	−480.780	129.986	at 400 K	
399	m-Xylene	C	4.12	85.49	−69.6458	15.0393	−89.4786	20.2488	0.11	0.353
		J	17.24	357.69	−291.398	62.9243	−374.379	84.7210	at 400 K	

Table I. (12. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
400	o-Xylene	C	4.54	84.31	−37.8568	14.2358	−82.2281	17.9778	0.09	0.295
		J	19.00	352.75	−158.393	59.5624	−344.042	75.2192		at 400 K
401	p-Xylene	C	4.29	84.23	−59.9201	14.4245	−80.5613	16.2887	0.12	0.398
		J	17.95	352.42	−250.706	60.3520	−337.068	68.1517		at 400 K
402	Propylbenzene	C	1.87	95.76	−93.6484	18.6798	−121.062	30.7663	0.08	0.278
		J	7.82	400.66	−391.825	78.1563	−506.524	128.726		at 400 K
403	Cumene	C	0.94	92.87	−113.201	19.5946	−132.744	35.4031	0.06	0.177
		J	3.93	388.57	−473.633	81.9839	−555.399	148.127		at 400 K
404	m-Ethyltoluene	C	−0.46	96.60	−78.1101	17.8991	−111.701	27.3003	0.10	0.337
		J	−1.92	404.17	−326.813	74.8899	−467.358	114.225		at 400 K
405	o-Ethyltoluene	C	0.29	95.42	−44.6124	16.9832	−102.249	23.7389	0.09	0.269
		J	1.21	399.24	−186.658	71.0576	−427.812	99.3236		at 400 K
406	p-Ethyltoluene	C	−0.78	95.34	−70.1543	17.3898	−104.487	24.1627	0.10	0.364
		J	−3.26	398.90	−293.526	72.7591	−437.173	101.097		at 400 K
407	1,2,3-Trimethyl-benzene	C	−2.29	91.98	−4.04318	14.3649	−65.5605	8.15073	0.13	0.398
		J	−9.58	384.84	−16.9167	60.1028	−274.305	34.1027		a 400 K
408	1,2,4-Trimethyl-benzene	C	−3.33	94.59	−11.3147	14.6736	−68.5618	9.00028	0.14	0.443
		J	−13.93	395.76	−47.3408	61.3943	−286.863	37.6572		at 400 K
409	Mesitylene	C	−3.84	92.09	−39.0839	15.5762	−78.8874	13.0492	0.13	0.428
		J	−16.07	385.30	−163.527	65.1710	−330.065	54.5979		at 400 K
410	Butylbenzene	C	−3.30	105.04	−97.5023	21.0204	−135.046	34.0540	0.08	0.280
		J	−13.81	439.49	−407.949	87.9494	−565.034	142.482		at 400 K
411	m-Diethylbenzene	C	−5.22	104.99	−83.7001	20.6034	−131.066	32.7307	0.09	0.286
		J	−21.84	439.28	−350.201	86.2048	−548.379	136.945		at 400 K
412	o-Diethylbenzene	C	−4.53	103.81	−51.9110	19.7999	−123.815	30.4597	0.08	0.245
		J	−18.95	434.34	−217.196	82.8429	−518.043	127.443		at 400 K
413	p-Diethylbenzene	C	−5.32	103.73	−73.9744	19.9886	−122.148	28.7705	0.10	0.318
		J	−22.26	434.01	−309.509	83.6324	−511.069	120.376		at 400 K
414	1,2,3,4-Tetra-methylbenzene	C	−10.02	99.55	11.6203	17.5132	−97.2955	20.4366	0.08	0.256
		J	−41.92	416.52	48.6592	73.2753	−407.084	85.5067		at 400 K
415	1,2,3,5-Tetra-methylbenzene	C	−10.71	100.99	13.7972	16.8311	−85.7482	15.0165	0.11	0.331
		J	−44.81	422.54	57.7276	70.4213	−358.770	62.8291		at 400 K
416	1,2,4,5-Tetra-methylbenzene	C	−10.82	100.03	43.9827	15.3638	−65.8206	6.42756	0.13	0.419
		J	−45.27	418.53	184.023	64.2823	−275.393	26.8929		at 400 K
417	Pentylbenzene	C	−8.23	114.47	−100.704	23.3498	−149.101	37.4718	0.09	0.292
		J	−34.43	478.94	−421.345	97.6955	−623.838	156.782		at 400 K
418	Pentamethyl-benzene	C	−17.80	106.09	−0.85140	20.9306	−128.591	31.6843	0.04	0.139
		J	−74.48	443.88	−3.56227	87.5734	−538.023	132.567		at 400 K
419	Hexylbenzene	C	−13.15	123.78	−104.384	25.7050	−163.627	41.1760	0.09	0.300
		J	−55.02	517.90	−436.742	107.550	−684.617	172.280		at 400 K
420	1,2,3-Triethyl-benzene	C	−16.25	121.23	−25.1242	22.7111	−127.941	26.8735	0.10	0.304
		J	−67.99	507.23	−105.120	95.0233	−535.304	112.439		at 400 K
421	1,2,4-Triethyl-benzene	C	−16.99	123.84	−32.3958	23.0198	−130.942	27.7230	0.11	0.338
		J	−71.09	518.15	−135.544	96.3148	−547.861	115.993		at 400 K
422	1,3,5-Triethyl-benzene	C	−17.86	121.34	−60.1650	23.9224	−141.268	31.7720	0.10	0.324
		J	−74.73	507.69	−251.730	100.091	−591.063	132.934		at 400 K
423	Hexamethyl-benzene	C	−25.26	108.12	8.17885	23.9982	−158.367	43.1246	0.03	0.070
		J	−105.69	452.37	34.2203	100.408	−662.606	180.433		at 400 K
424	1-Phenylheptane	C	−18.08	133.09	−106.566	27.9693	−176.470	43.8926	0.09	0.296
		J	−75.65	556.85	−445.872	117.024	−738.349	183.646		at 400 K

Table I. (13. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
425	1-Phenyloctane	C	−23.00	142.40	−109.020	30.2459	−189.435	46.6376	0.09	0.298
		J	−96.23	595.80	−456.140	126.549	−792.597	195.132		at 400 K
426	1,2,3,4-Tetra-ethylbenzene	C	−29.46	138.55	−16.4878	28.6415	−180.469	45.4003	0.07	0.204
		J	−123.26	579.69	−68.9849	119.836	−755.082	189.955		at 400 K
427	1,2,3,5-Tetraethyl-benzene	C	−29.36	139.99	−14.3108	27.9593	−168.922	39.9802	0.08	0.253
		J	−122.84	585.72	−59.8765	116.982	−706.768	167.277		at 400 K
428	1,2,4,5-Tetraethyl-benzene	C	−29.46	139.03	47.2557	25.0790	−128.789	22.1476	0.14	0.457
		J	−123.26	581.70	197.718	104.930	−538.854	92.6656		at 400 K
429	1-Phenylnonane	C	−27.93	151.71	−113.374	32.6453	−204.856	50.8877	0.09	0.305
		J	−116.86	634.75	−474.358	136.588	−857.117	212.914		at 400 K
430	1-Phenyldecane	C	−32.86	161.02	−115.612	34.9109	−217.649	53.5483	0.09	0.296
		J	−137.49	673.71	−483.719	146.067	−910.642	224.046		at 400 K
431	Pentaethyl-benzene	C	−41.87	154.84	−35.9865	34.8409	−232.558	62.8889	0.06	0.127
		J	−175.18	647.85	−150.567	145.774	−973.021	263.127		at 400 K
432	1-Phenylundecane	C	−37.78	170.32	−117.855	37.1768	−230.464	56.2301	0.09	0.295
		J	−158.07	712.62	−493.106	115.548	−964.260	235.267		at 400 K
433	1-Phenyldodecane	C	−42.71	179.63	−122.490	39.5932	−246.197	60.6505	0.09	0.302
		J	−178.70	751.57	−512.498	165.658	−1030.09	253.762		at 400 K
434	Hexaethyl-benzene	C	−53.60	166.62	−33.9832	40.6906	−283.127	80.5701	0.05	0.129
		J	−224.26	697.14	−142.186	170.249	−1184.60	337.105		at 300 K
435	1-Phenyltridecane	C	−47.63	188.94	−124.664	41.8527	−258.850	63.2253	0.09	0.302
		J	−199.28	790.52	−521.592	175.112	−1083.03	264.534		at 400 K
436	1-Phenyltetra-decane	C	−52.56	198.25	−126.565	44.0999	−271.380	65.7716	0.09	0.299
		J	−219.91	829.48	−529.548	184.514	−909.517	275.188		at 400 K
437	1-Phenylpenta-decane	C	−57.99	207.56	−131.261	46.5179	−287.086	70.1571	0.09	0.306
		J	−240.54	868.43	−549.197	194.631	−1201.17	293.537		at 400 K
438	1-Phenylhexa-decane	C	−62.41	216.87	−133.505	48.7838	−299.901	72.8389	0.09	0.305
		J	−261.12	907.38	−558.585	204.111	−1254.79	304.758		at 400 K
439	Styrene	C	35.22	82.48	−88.1869	15.8975	−115.890	33.6517	0.05	0.164
		J	147.36	345.10	−368.974	66.5153	−484.883	140.799		at 400 K
440	α-Methylstyrene	C	27.00	91.70	−58.1114	16.5570	−108.180	28.1957	0.08	0.251
		J	112.97	383.67	−243.138	69.2746	−452.624	117.971		at 400 K
441	Propenylbenzene, cis	C	29.00	91.70	−58.1111	16.5570	−108.180	28.1957	0.08	0.251
		J	121.34	383.67	−243.137	69.2744	−452.622	117.970		at 400 K
442	Propenylbenzene, trans	C	28.00	90.90	−70.098	17.2792	−117.791	31.9939	0.06	0.233
		J	117.15	380.33	−293.292	72.2963	−492.836	133.862		at 400 K
443	m-Methylstyrene	C	27.60	93.10	−58.1111	16.5570	−108.179	28.1956	0.08	0.251
		J	115.48	389.53	−243.137	69.2744	−452.622	117.970		at 400 K
444	p-Methylstyrene	C	28.30	91.70	−58.1111	16.5570	−108.179	28.1956	0.08	0.251
		J	118.41	383.67	−243.137	69.2744	−452.622	117.970		at 400 K
445	p-Methylstyrene	C	27.40	91.70	−58.1111	16.5570	−108.179	28.1956	0.08	0.251
		J	114.64	383.67	−243.137	69.2744	−452.622	117.970		at 400 K
446	Naphthalene	C	36.08	80.22	−148.490	19.4731	−141.927	40.4168	0.06	0.214
		J	150.96	335.64	−621.280	81.4754	−593.822	169.104		at 400 K
447	1-Methyl-naphthalene	C	27.93	90.21	−142.641	21.8966	−158.609	45.1022	0.05	0.180
		J	116.86	377.44	−596.812	91.6152	−663.618	188.708		at 400 K
448	2-Methyl-naphthalene	C	27.75	90.83	−124.240	21.0150	−147.874	40.997	0.05	0.198
		J	116.11	380.03	−519.819	87.9270	−618.705	171.531		at 400 K
449	1-Ethyl-naphthalene	C	23.10	99.94	−152.422	24.8302	−181.922	52.6424	0.04	0.155
		J	96.65	418.15	−637.733	103.890	−761-161	220.256		at 400 K
450	2-Ethyl-naphthalene	C	22.92	100.56	−134.020	23.9487	−171.187	48.5367	0.05	0.171
		J	95.90	420.74	−560.740	100.201	−716.251	203.078		at 400 K

Table I. (14. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
451	1,2-Dimethyl-naphthalene	C	19.97	97.23	−142.030	24.3566	−175.012	49.4535	0.05	0.182
		J	83.55	406.81	−594.255	101.908	−732.254	206.914		at 400 K
452	1,3-Dimethyl-naphthalene	C	19.55	97.86	−123.628	23.4750	−164.278	45.3483	0.05	0.198
		J	81.80	409.45	−517.262	98.2198	−687.340	189.738		at 400 K
453	1,4-Dimethyl-naphthalene	C	19.72	95.86	−142.030	24.3566	−175.012	49.4535	0.05	0.182
		J	82.51	401.08	−594.255	101.908	−732.254	206.914		at 400 K
454	1,5-Dimethyl-naphthalene	C	19.55	95.86	−142.030	24.3566	−175.012	49.4535	0.05	0.182
		J	81.80	401.08	−594.255	101.908	−732.254	206.914		at 400 K
455	1,6-Dimethyl-naphthalene	C	19.72	97.86	−123.628	23.4750	−164.278	45.3483	0.05	0.198
		J	82.51	409.45	−517.262	98.2198	−687.340	189.738		at 400 K
456	1,7-Dimethyl-naphthalene	C	19.55	97.86	−123.628	23.4750	−164.278	45.3483	0.05	0.198
		J	81.80	409.45	−517.262	98.2198	−687.340	189.738		at 400 K
457	2,3-Dimethyl-naphthalene	C	19.97	98.22	−76.5168	21.1683	−134.549	33.2712	0.07	0.231
		J	83.55	410.95	−320.148	88.5683	−562.955	139.207		at 400 K
458	2,6-Dimethyl-naphthalene	C	19.72	97.68	−95.7439	22.3642	−152.158	41.2287	0.07	0.182
		J	82.51	408.69	−400.594	93.5720	−636.630	172.501		at 400 K
459	2,7-Dimethyl-naphthalene	C	19.72	97.68	−93.9111	22.2821	−150.989	40.6956	0.06	0.195
		J	82.51	408.69	−392.924	93.2285	−631.738	170.270		at 400 K
460	1-Propyl-naphthalene	C	17.85	109.55	−143.861	26.6555	−188.511	52.5299	0.06	0.208
		J	74.68	458.36	−601.917	111.527	−788.735	219.786		at 400 K
461	2-Propyl-naphthalene	C	17.65	110.18	−126.963	25.8372	−178.477	48.5915	0.06	0.163
		J	73.85	460.99	−531.215	108.103	−746.752	203.307		at 400 K
462	2-Ethyl-3-methyl-naphthalene	C	15.72	109.33	−82.9244	23.8972	−154.215	38.7991	0.06	0.162
		J	65.77	457.44	−346.956	99.9859	−654.235	162.335		at 400 K
463	2-Ethyl-6-methyl-naphthalene	C	14.65	108.79	−188.816	30.3922	−268.639	99.4777	0.64	0.713
		J	61.30	455.18	−790.006	127.161	−1123.98	416.214		at 400 K
464	2-Ethyl-7-methyl-naphthalene	C	14.65	108.79	−188.816	30.3922	−268.639	99.4777	0.64	0.713
		J	61.30	455.18	−790.006	127.161	−1123.98	416.214		at 400 K
465	1-Butyl-naphthalene	C	12.68	118.83	−146.530	28.9328	−201.627	55.4257	0.07	0.228
		J	53.05	497.18	−613.083	121.055	−843.609	231.901		at 400 K
466	2-Butyl-naphthalene	C	12.50	119.46	−125.298	27.8751	−187.492	49.3400	0.06	0.180
		J	52.30	499.82	−524.247	116.629	−784.466	206.438		at 400 K
467	1-Pentyl-naphthalene	C	7.75	128.26	−153.320	31.4642	−218.854	60.4203	0.06	0.220
		J	32.43	536.64	−641.489	131.646	−915.686	252.798		at 400 K
468	2-Pentyl-naphthalene	C	7.57	128.89	−132.806	30.4623	−205.994	55.1363	0.05	0.174
		J	31.67	539.28	−555.661	127.454	−861.880	230.690		at 400 K
469	Spiropentane	C	44.27	67.45	−99.1311	12.8757	−91.4187	26.0775	0.08	0.286
		J	185.23	282.21	−414.764	53.8720	−382.496	109.108		at 400 K
470	1,3,5-Cyclo-heptatriene	C	43.47	75.44	−102.024	16.3974	−130.799	41.6292	0.04	0.074
		J	181.88	315.64	−426.869	68.6066	−547.263	174.176		at 900 K
471	Ethynylbenzene	C	78.22	76.88	−91.5779	15.7443	−128.254	41.1621	0.04	0.081
		J	327.27	321.67	−383.162	65.8740	−536.615	172.222		at 900 K
472	1,3,5,7-Cyclooctatetraene	C	71.23	78.10	−99.5823	16.3613	−119.421	34.6178	0.11	0.376
		J	298.03	326.77	−416.652	68.4558	−499.658	144.841		at 400 K
473	Azulene	C	66.90	80.75	−173.684	20.1827	−149.130	42.9011	0.06	0.231
		J	279.91	337.86	−726.696	84.4446	−623.959	179.498		at 400 K
474	Decahydro-naphthalene, cis	C	−40.38	90.28	−262.199	26.4227	−153.598	32.4075	0.18	0.578
		J	−168.95	377.73	−1097.04	110.553	−642.652	135.593		at 400 K
475	Decahydro-naphthalene, trans	C	−43.57	89.52	−233.276	24.9481	−130.801	21.4460	0.20	0.355
		J	−182.30	374.55	−976.025	104.383	−547.272	89.7301		at 500 K
476	Biphenyl	C	43.52	93.85	−210.472	25.3666	−195.274	58.6573	0.06	0.188
		J	182.09	392.67	−880.613	106.134	−817.025	245.422		at 400 K

Table I. (cont.)

CARBON, HYDROGEN AND OXYGEN COMPOUNDS

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
501	Methyl ether	C	−43.99	63.83	47.9702	3.85380	−5.16360	−4.40920	0.15	0.439
		J	−184.05	267.06	200.707	16.1243	−21.6045	−18.4481		at 400 K
502	Ethyl methyl ether	C	−51.73	74.24	57.2387	5.64464	−11.3160	−4.71049	0.14	0.422
		J	−216.44	310.62	239.487	23.6172	−47.3462	−19.7087		at 400 K
503	Ethyl ether	C	−60.28	81.90	53.3849	7.98526	−25.3001	−1.42287	0.13	0.394
		J	−252.21	342.67	223.362	33.4103	−105.856	−5.95328		at 400 K
504	Methyl propyl ether	C	−56.82	83.52	53.3849	7.98526	−25.3001	−1.4228	0.13	0.394
		J	−237.73	349.45	223.362	33.4103	−105.856	−5.95328		at 400 K
505	Methyl isopropyl ether	C	−60.24	80.86	34.5303	8.73028	−33.9344	2.21729	0.12	0.352
		J	−252.04	338.32	144.474	36.5275	−141.981	9.27712		at 400 K
506	Methyl tert-butyl ether	C	−70.00	84.36	10.6850	12.0574	−58.9993	8.89489	0.23	0.613
		J	−292.88	352.96	44.7057	50.4482	−246.853	37.2162		at 400 K
507	Propyl ether	C	−70.00	100.98	47.8415	12.5891	−52.3784	4.82663	0.12	0.359
		J	−292.88	422.50	200.169	52.6727	−219.151	20.1946		at 400 K
508	Isopropyl ether	C	−76.20	93.27	47.8415	12.5891	−52.3784	4.82663	0.12	0.359
		J	−318.82	390.24	200.169	52.6727	−219.151	20.1946		at 400 K
509	Isopropyl tert-butyl ether	C	−85.60	99.89	49.7011	14.7090	−63.7379	7.17517	0.15	0.421
		J	−358.15	417.94	207.950	61.5426	−266.679	30.0209		at 400 K
510	Butyl ether	C	−79.80	119.60	41.4890	17.2390	−80.3252	11.5881	0.11	0.352
		J	−333.88	500.41	173.590	72.1282	−336.081	48.4848		at 400 K
511	sec-Butyl ether	C	−86.20	110.57	41.4890	17.2390	−80.3252	11.5881	0.11	0.352
		J	−360.66	462.62	173.590	72.1282	−336.081	48.4848		at 400 K
512	tert-Butyl ether	C	−87.20	102.12	41.4890	17.2390	−80.3252	11.5881	0.11	0.352
		J	−364.84	427.27	173.590	72.1282	−336.081	48.4848		at 400 K
513	Ethylene oxide	C	−12.58	57.94	−17.9619	5.30677	−30.0067	6.18902	0.15	0.505
		J	−52.63	242.42	−75.1526	22.2035	−125.548	25.8949		at 400 K
514	Propylene oxide	C	−22.17	68.53	−18.7772	7.71386	−46.5739	11.0891	0.10	0.340
		J	−92.76	286.73	−78.5638	32.2748	−194.865	46.3966		at 400 K
515	Furan	C	−8.29	63.86	−84.8425	10.3213	−82.4936	25.6554	0.07	0.207
		J	−34.69	267.19	−354.981	43.1843	−345.153	107.342		at 400 K
516	p-Dioxone	C	−75.30	71.65	−86.4367	12.3653	−69.0906	12.0565	0.31	0.997
		J	−315.06	299.78	−361.651	51.7362	−289.075	50.4442		at 400 K
517	Methanol	C	−48.08	57.29	50.5146	1.69268	6.17571	−6.80664	0.24	0.684
		J	−201.17	239.70	211.353	7.08219	25.8392	−28.4790		at 400 K
518	Ethyl alcohol	C	−56.12	67.54	13.5801	5.62403	−30.0661	6.33049	0.15	0.456
		J	−234.81	282.59	56.8192	23.5309	−125.797	26.4868		at 400 K
519	Propyl alcohol	C	−61.55	77.63	21.3401	7.19721	−32.8382	4.63536	0.13	0.406
		J	−257.53	324.80	89.2869	30.1131	−137.395	19.3943		at 400 K
520	Isopropyl alcohol	C	−65.15	74.07	−17.3480	9.41971	−63.4070	17.7604	0.16	0.578
		J	−272.59	309.91	−72.5842	39.4121	−265.295	74.3094		at 400 K
521	Butyl alcohol	C	−65.59	86.80	18.9468	9.47791	−46.0132	7.56913	0.12	0.391
		J	−274.43	363.17	79.2735	39.6556	−192.519	31.6692		at 400 K
522	sec-Butyl alcohol	C	−69.86	85.81	13.9114	10.2096	−57.5167	12.6306	0.12	0.399
		J	−292.29	359.03	58.2054	42.7169	−240.650	52.8465		at 400 K
523	tert-Butyl alcohol	C	−77.87	77.98	−10.9726	11.5006	−74.6090	19.8468	0.07	0.227
		J	−325.81	326.27	−45.9092	48.1184	−312.164	83.0391		at 400 K

Table 1. (1. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
524	Pentyl alcohol	C	−72.27	96.21	16.5536	11.7586	−59.1879	10.5028	0.12	0.381
		J	−302.38	402.54	69.2601	49.1979	−247.642	43.9438		at 400 K
525	tert-Pentyl alcohol	C	−78.65	87.68	−22.5584	13.4797	−78.4851	17.2329	0.21	0.593
		J	−329.07	366.85	−94.3843	56.3991	−328.382	72.1025		at 400 K
526	Hexyl alcohol	C	−76.39	105.52	14.1604	14.0393	−72.3629	13.4366	0.11	0.374
		J	−319.62	441.50	59.2468	58.7403	−302.766	56.2186		at 400 K
527	Heptyl alcohol	C	−80.03	114.83	11.7671	16.3200	−85.5379	16.3704	0.11	0.369
		J	−334.85	480.45	49.2335	68.2827	−357.890	68.4934		at 400 K
528	Octyl alcohol	C	−85.34	124.14	9.37388	18.6007	−98.7129	19.3041	0.11	0.365
		J	−357.06	519.40	39.2202	77.8251	−413.014	80.7682		at 400 K
529	Nonyl alcohol	C	−92.47	133.45	6.98062	20.8814	−111.888	22.2379	0.11	0.361
		J	−386.89	558.35	29.2069	87.3675	−468.138	93.0430		at 400 K
530	Decyl alcohol	C	−96.38	142.76	4.58736	23.1621	−125.063	25.1716	0.11	0.359
		J	−403.25	597.31	19.1935	96.9100	−523.262	105.318		at 400 K
531	Undecyl alcohol	C	−100.91	152.07	2.19410	25.4428	−138.238	28.1054	0.11	0.357
		J	−422.21	636.26	9.18012	106.453	−578.387	117.593		at 400 K
532	Dodecyl alcohol	C	−105.84	161.38	−0.19916	27.7235	−151.413	31.0392	0.10	0.355
		J	−442.83	675.21	−0.83327	115.995	−633.512	129.868		at 400 K
533	1-Tridecanol	C	−110.77	170.37	−7.59032	30.2809	−169.436	36.6154	0.10	0.343
		J	−463.46	712.83	−31.7579	126.695	−708.918	153.198		at 400 K
534	1-Tetradecanol	C	−115.70	179.68	−10.0445	32.5575	−182.401	39.3604	0.10	0.342
		J	−484.09	751.78	−42.0263	136.220	−763.166	164.684		at 400 K
535	1-Pentadecanol	C	−120.62	188.99	−11.9460	34.8046	−194.931	41.9067	0.10	0.335
		J	−504.67	790.73	−49.9819	145.622	−815.589	175.337		at 400 K
536	1-Hexadecanol	C	−125.54	198.30	−16.6423	37.2226	−210.637	46.2922	0.10	0.341
		J	−525.26	829.69	−69.6313	155.739	−881.304	193.686		at 400 K
537	1-Heptadecanol	C	−130.47	207.61	−18.6052	39.4714	−223.139	48.8037	0.10	0.337
		J	−545.89	868.64	−77.8444	165.148	−933.614	204.194		at 400 K
538	1-Octadecanol	C	−135.39	216.92	−20.7873	41.7356	−235.982	51.5203	0.10	0.333
		J	−566.47	907.59	−86.9743	174.622	−987.347	215.561		at 400 K
539	1-Nonadecanol	C	−140.32	226.23	−25.4136	44.1473	−251.526	55.7988	0.10	0.338
		J	−587.10	946.55	−106.330	184.712	−1052.38	233.462		at 400 K
540	1-Eicosanol	C	−145.25	235.54	−30.0398	46.5590	−267.070	60.0774	0.10	0.343
		J	−607.73	985.50	−125.687	194.802	−1117.42	251.363		at 400 K
541	Allyl alcohol	C	−31.55	73.51	−2.63664	7.51386	−48.5174	12.7086	0.06	0.142
		J	−132.01	307.57	−11.0317	31.4380	−202.997	53.1726		at 400 K
542	Ethylene glycol	C	−93.05	77.33	69.8659	6.87960	−53.6543	17.6408	0.26	0.499
		J	−389.32	323.55	292.318	28.7842	−224.490	73.8092		at 800 K
543	Cyclohexanol	C	−70.40	78.32	−100.671	15.7112	−74.9334	8.95188	0.17	0.535
		J	−294.55	327.69	−421.207	65.7354	−313.521	37.4546		at 400 K
544	Formaldehyde	C	−27.70	52.29	63.0609	0.44175	11.4453	−7.37248	0.19	0.557
		J	−115.90	218.78	263.847	1.84827	47.8872	−30.8465		at 400 K
545	Acetaldehyde	C	−39.76	63.15	36.9463	3.45322	−10.3300	−0.95573	0.13	0.402
		J	−166.36	264.22	154.583	14.4483	−43.2209	−3.99877		at 400 K
546	Propionaldehyde	C	−45.90	72.83	27.9909	6.24296	−31.0390	5.07665	0.06	0.171
		J	−192.05	304.72	117.114	26.1205	−129.867	21.2407		at 400 K
547	Butyraldehyde	C	−49.00	82.44	33.6254	8.25556	−41.1432	6.89389	0.08	0.142
		J	−205.02	344.93	140.689	34.5413	−172.143	28.8440		at 400 K

Table I. (2. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
548	Valeraldehyde	C	−54.45	91.53	34.0083	10.3335	−50.3183	7.55102	0.09	0.181
		J	−227.82	382.96	142.291	43.2354	−210.532	31.5934		at 400 K
549	Hexanal	C	−59.37	101.07	28.2373	12.8285	−67.7382	13.0146	0.09	0.300
		J	−248.40	422.88	118.144	53.6743	−283.417	54.4529		at 400 K
550	Heptanal	C	−63.10	110.34	25.088	15.1414	−81.1268	15.8724	0.08	0.215
		J	−264.01	461.66	104.968	63.3516	−339.435	66.4100		at 400 K
551	Octanal	C	−69.23	119.66	25.2955	17.2573	−91.2527	17.1276	0.08	0.266
		J	−289.66	500.66	105.836	72.2045	−381.801	71.6620		at 400 K
552	Nonanal	C	−74.16	128.97	19.6305	19.7241	−107.758	21.9005	0.11	0.338
		J	−310.29	539.61	82.1336	82.5255	−450.860	91.6314		at 400 K
553	Decanal	C	−79.09	138.28	16.3753	22.0652	−122.061	25.4490	0.08	0.274
		J	−330.91	578.56	68.5139	92.3208	−510.704	106.479		at 400 K
554	Acetone	C	−52.00	70.49	33.3866	5.41177	−17.8317	−0.50376	0.15	0.454
		J	−217.57	294.93	139.689	22.6328	−74.6080	−2.10772		at 400 K
555	2-Butanone	C	−56.97	80.81	57.4339	7.08230	−26.1433	0.87469	0.14	0.453
		J	−238.36	338.11	240.303	29.6323	−109.384	3.65968		at 400 K
556	2-Pentanone	C	−61.82	89.91	2.73937	11.4727	−67.2992	15.9102	0.01	0.017
		J	−258.65	376.18	11.4615	48.0020	−281.580	66.5681		at 300 K
557	Ketene	C	−14.60	57.79	47.4912	3.23379	−25.0958	8.26863	0.07	0.154
		J	−61.09	241.79	198.703	13.5301	−105.001	34.5959		at 400 K
558	Cyclohexanone	C	−55.00	77.00	−90.2797	13.2282	−46.6438	−3.66316	0.17	0.518
		J	−230.12	322.17	−377.730	55.3466	−195.158	−15.3267		at 400 K
559	Formic acid	C	−90.49	59.45	27.9756	3.24215	−20.0869	4.81604	0.09	0.246
		J	−378.61	248.74	117.050	13.5652	−84.0437	20.1503		at 600 K
560	Acetic acid	C	−103.93	67.52	11.5623	6.08567	−41.8646	11.8218	0.09	0.194
		J	−434.84	282.50	48.3767	25.4624	−175.161	49.4624		at 700 K
561	Methyl formate	C	−83.60	72.00	12.6503	6.01761	−40.4770	11.0023	0.15	0.324
		J	−349.78	301.25	52.9287	25.1777	−169.356	46.0334		at 400 K
562	Acetic anhydride	C	−137.60	93.20	−55.7638	12.2429	−88.1118	25.3328	0.09	0.223
		J	−575.72	389.95	−233.316	51.2241	−368.660	105.992		at 700 K
563	Ethyl acetate	C	−105.86	86.70	58.9779	7.84435	−23.5139	−4.87477	0.35	0.470
		J	−442.92	362.75	246.763	32.8207	−98.3821	−20.3960		at 600 K
564	Acrylic acid	C	−80.36	75.29	4.16262	7.61929	−56.1674	16.6606	0.07	0.176
		J	−336.23	315.01	17.4164	31.8790	−235.004	69.708		at 700 K
565	Phenol	C	−23.03	75.43	−85.5920	14.2846	−115.250	36.4646	0.04	0.080
		J	−96.36	315.60	−358.117	59.7665	−482.206	152.568		at 500 K
566	m-Cresol	C	−31.63	85.27	−110.277	17.5199	−147.196	51.5023	0.21	0.793
		J	−132.34	356.77	−461.400	73.3031	−615.869	215.486		at 300 K
567	o-Cresol	C	−30.47	85.47	−62.1508	16.0015	−130.116	45.1051	0.10	0.298
		J	−127.49	357.61	−260.039	66.9501	−544.405	188.719		at 400 K
568	p-Cresol	C	−29.97	83.09	−88.9770	16.5306	−133.584	45.5479	0.10	0.300
		J	−125.39	347.65	−372.280	69.1641	−558.916	190.572		at 400 K
569	Benzoic acid	C	−69.36	88.19	−91.7748	13.6212	−81.1634	16.3601	0.30	0.901
		J	−290.20	368.99	−383.985	56.9908	−339.588	68.4504		at 400 K

Table I. (cont.)

NITROGEN COMPOUNDS

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
601	Methylamine	C	−5.50	57.98	38.4542	2.90161	−5.44728	−2.17126	0.14	0.425
		J	−23.01	242.59	160.892	12.1403	−22.7914	−9.08454		at 400 K
602	Ethylamine	C	−11.00	68.08	8.81493	6.57066	−37.8077	9.09415	0.06	0.216
		J	−46.02	284.85	36.8817	27.4916	−158.187	38.0493		at 400 K
603	Propylamine	C	−17.30	77.48	15.9821	8.35408	−43.5086	8.56400	0.09	0.319
		J	−72.38	324.18	66.8690	34.9535	−182.040	35.8318		at 400 K
604	Butylamine	C	−22.00	86.76	12.1282	10.6947	−57.4927	11.8516	0.09	0.313
		J	−92.05	363.00	50.7444	44.7466	−240.549	49.5872		at 400 K
605	sec-Butylamine	C	−24.90	83.90	7.25383	10.5723	−49.6477	5.78014	0.09	0.192
		J	−104.18	351.04	30.3500	44.2346	−207.723	24.1841		at 900 K
606	tert-Butylamine	C	−28.65	80.76	−27.9974	12.8597	−84.3362	22.3132	0.09	0.310
		J	−119.87	337.90	−117.141	53.8051	−352.863	93.3585		at 400 K
607	Dimethylamine	C	−4.50	65.24	−0.40548	6.43768	−31.7522	5.58751	0.15	0.464
		J	−18.83	272.96	−1.69654	26.9352	−132.851	23.3781		at 400 K
608	Diethylamine	C	−17.30	84.18	4.86855	10.5802	−52.1327	8.72360	0.13	0.414
		J	−72.38	352.21	20.3700	44.2677	−218.123	36.4995		at 400 K
609	Trimethylamine	C	−5.70	69.02	−19.5966	9.48592	−52.9888	11.0384	0.15	0.469
		J	−23.85	288.78	−81.9922	39.6891	−221.705	46.1848		at 400 K
610	Triethylamine	C	−23.80	96.90	−9.42204	15.5034	−81.9402	15.5895	0.16	0.529
		J	−99.58	405.43	−39.4218	64.8663	−342.837	65.2263		at 400 K
611	Ethyleneimine	C	29.50	59.90	−49.6036	7.21785	−49.2621	13.4848	0.11	0.368
		J	123.43	250.62	−207.541	30.1994	−206.113	56.4204		at 400 K
612	Pyrrolidine	C	−0.86	73.97	−120.084	12.6165	−75.4361	17.0866	0.16	0.551
		J	−3.60	309.49	−502.430	52.7875	−315.624	71.4903		at 400 K
613	Pyridine	C	33.50	67.59	−95.0238	11.7649	−84.9656	23.9807	0.09	0.304
		J	140.16	282.80	−397.579	49.2244	−355.496	100.335		at 400 K
614	2-Picoline	C	23.65	77.68	−84.6290	13.2476	−87.1791	22.4875	0.09	0.306
		J	98.95	325.01	−354.088	55.4278	−364.757	94.0876		at 400 K
615	3-Picoline	C	25.37	77.67	−86.2232	13.2691	−87.2808	22.4247	0.09	0.326
		J	106.15	324.97	−360.758	55.5176	−365.183	93.8248		at 400 K
616	Aniline	C	20.76	76.28	−96.7496	15.2444	−122.579	39.0063	0.04	0.079
		J	86.86	319.16	−404.800	63.7824	−512.871	163.202		at 500 K
617	Acetonitrile	C	21.00	58.19	48.9068	2.85671	−10.7318	0.76457	0.07	0.200
		J	87.86	243.47	204.626	11.9525	−44.9020	3.19895		at 400 K
618	Acrylonitrile	C	44.20	65.47	25.5381	5.27235	−37.3852	10.99308	0.03	0.049
		J	184.93	273.93	106.851	22.0595	−156.420	45.9950		at 700 K
619	Propionitrile	C	12.10	68.50	36.7805	5.36207	−26.2715	4.66598	0.06	0.170
		J	50.63	286.60	153.889	22.4349	−109.920	19.5225		at 400 K
620	Butyronitrile	C	8.14	77.78	36.3251	7.65734	−39.1219	7.12405	0.07	0.240
		J	34.06	325.43	151.9838	32.0383	−163.686	29.8070		at 400 K
621	Isobutyronitrile	C	6.07	74.88	14.6566	8.69771	−53.0477	12.9999	0.05	0.143
		J	25.40	313.30	61.3231	36.3911	−221.952	54.3913		at 400 K
622	Benzonitrile	C	52.30	76.73	−61.1978	13.6477	−105.189	31.9209	0.05	0.100
		J	218.82	321.04	−256.052	57.1017	−440.109	133.557		at 400 K
623	Nitromethane	C	−17.86	65.73	17.7249	4.72298	−25.8257	4.97929	0.10	0.303
		J	−74.73	275.01	74.1606	19.7609	−108.550	20.8333		at 400 K

Table I. (1. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
624	Nitroethane	C	−24.20	75.39	−14.5813	8.27846	−55.5934	14.9272	0.07	0.237
		J	−101.25	315.43	−61.0082	34.6370	−232.603	62.4551		at 400 K
625	1-Nitropropane	C	−29.80	85.00	−6.08516	10.1127	−62.4407	14.9655	0.09	0.290
		J	−124.68	355.64	−25.4603	42.3114	−261.252	62.6155		at 400 K
626	2-Nitropropane	C	−33.50	83.10	−27.7536	11.1530	−76.3664	20.8413	0.06	0.200
		J	−140.16	347.69	−116.121	46.6642	−319.517	87.1997		at 400 K
627	1-Nitrobutane	C	−34.40	94.28	−9.93902	12.4533	−76.4245	18.2531	0.09	0.290
		J	−143.93	394.47	−41.5849	52.1045	−319.761	76.3708		at 400 K
628	2-Nitrobutane	C	−39.10	91.62	−28.7935	13.1983	−85.0590	21.8932	0.08	0.253
		J	−163.59	383.34	−120.472	55.2216	−355.887	91.6021		at 400 K
629	Methyl nitrite	C	−15.30	67.95	30.1091	4.81232	−26.9874	5.36383	0.08	0.249
		J	−64.02	284.30	125.976	20.1347	−112.915	22.4422		at 400 K
630	Methyl nitrate	C	−28.80	72.15	40.7654	5.75272	−35.7540	8.33428	0.05	0.138
		J	−120.50	301.88	170.562	24.0694	−149.595	34.8706		at 400 K
631	Ethyl nitrate	C	−36.80	83.25	8.45928	9.30821	−65.5217	18.2821	0.04	0.123
		J	−153.97	348.32	35.3935	38.9454	−274.142	76.4923		at 400 K
632	Propyl nitrate	C	−41.60	92.10	16.9555	11.1424	−72.3688	18.3204	0.06	0.191
		J	−174.05	385.35	70.9414	46.6197	−302.791	76.6526		at 400 K
633	Isopropyl nitrate	C	−45.65	89.20	−4.71306	12.1828	−86.2949	24.1963	0.05	0.114
		J	−191.00	373.21	−19.7194	50.9727	−361.058	101.237		at 400 K

Table I. (cont.)

HALOGEN COMPOUNDS

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
701	Fluoromethane	C	−55.90	53.25	40.4618	1.55846	4.52688	−5.74336	0.24	0.240
		J	−233.89	222.80	169.292	6.52060	18.9405	−24.0302		at 900 K
702	Difluoromethane	C	−108.24	58.94	29.4025	2.76205	−10.8355	0.18488	0.18	0.381
		J	−452.88	246.60	123.020	11.5773	−45.3358	0.77353		at 400 K
703	Trifluoromethane	C	−166.71	62.04	9.19947	4.96457	−43.8303	14.9999	0.33	0.661
		J	−697.51	259.58	38.4904	20.7717	−183.386	62.7593		at 500 K
704	Carbon tetrafluoride	C	−223.00	62.50	19.5162	5.68660	−52.8349	17.9365	0.07	0.141
		J	−933.03	261.50	81.6554	23.7927	−221.061	75.0464		at 700 K
705	Fluoroethane	C	−62.50	63.32	11.0978	5.06102	−24.9140	4.15875	0.12	0.362
		J	−261.50	264.51	46.4332	21.1753	−104.240	17.4002		at 400 K
706	1,1-Difluoro-ethane	C	−118.00	67.52	12.9397	6.17654	−42.6513	12.1713	0.15	0.451
		J	−493.71	282.50	54.1394	25.8426	−178.453	50.9248		at 700 K
707	1,1,1-Trifluoro-ethane	C	−178.20	68.66	13.6960	7.50280	−62.0435	20.1072	0.04	0.067
		J	−745.59	287.27	57.3038	31.3916	−259.590	84.1282		at 900 K
708	Hexafluoroethane	C	−321.00	79.73	34.1448	10.0138	−98.2938	34.5525	0.09	0.154
		J	−1343.06	332.08	142.861	41.8978	−411.261	144.567		at 900 K
709	1-Fluoropropane	C	−67.20	72.71	17.7695	6.94365	−32.3577	4.48312	0.14	0.452
		J	−281.16	304.22	74.3475	29.0522	−135.385	18.7699		at 400 K
710	2-Fluoropropane	C	−69.00	69.82	−3.89897	7.98402	−46.2837	10.3619	0.11	0.339
		J	−288.70	292.13	−16.3133	33.4051	−193.651	43.3543		at 400 K
711	Octafluorocyclo-butane	C	−365.20	95.69	21.6050	15.8904	−153.745	54.2171	0.11	0.293
		J	−1528.00	400.37	90.3948	66.4854	−643.268	226.845		at 500 K

Table I. (1. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
712	1,1-Difluoro-ethylene	C	−82.50	63.38	7.78281	5.81931	−49.8528	16.6371	0.09	0.131
		J	−345.18	265.18	32.5632	24.3480	−208.584	69.6093		at 300 K
713	Trifluoroethylene	C	−118.50	69.94	39.5965	5.47749	−46.6213	15.1265	0.04	0.060
		J	−495.80	292.63	165.671	22.9178	−195.063	63.2893		at 400 K
714	Tetrafluoro-ethylene	C	−157.40	71.69	69.0914	5.44769	−48.7591	16.2463	0.06	0.145
		J	−658.56	299.95	289.078	22.7931	−204.008	76.9743		at 400 K
715	Fluorobenzene	C	−27.86	72.33	−91.7233	13.5038	−105.424	32.1433	0.05	0.141
		J	−116.57	302.63	−383.770	56.4999	−441.095	134.488		at 400 K
716	m-Difluoro-benzene	C	−74.09	76.57	−63.8750	13.6615	−110.911	34.6320	0.04	0.076
		J	−309.99	320.37	−267.253	57.1598	−464.051	144.900		at 700 K
717	o-Difluorobenzene	C	−70.39	76.94	−58.5159	13.3627	−105.668	32.6198	0.03	0.071
		J	−294.51	321.92	−244.831	55.9095	−442.114	136.481		at 500 K
718	p-Difluorobenzene	C	−73.43	75.43	−61.7201	13.6544	−111.511	35.1409	0.03	0.065
		J	−307.23	315.60	−258.237	57.1299	−466.562	147.029		at 500 K
719	Hexafluorobenzene	C	−228.64	91.59	86.3911	12.5954	−108.795	34.8520	0.04	0.082
		J	−956.63	383.21	361.460	52.6990	−455.197	145.821		at 400 K
720	α, α, α-Trifluoro-toluene	C	−143.42	89.05	−96.5126	17.4773	−139.927	43.2606	0.05	0.119
		J	−600.07	372.59	−403.809	73.1248	−585.454	181.002		at 400 K
721	p-Fluorotoluene	C	−35.38	81.15	−80.2709	14.8859	−105.648	29.6467	0.06	0.220
		J	−148.03	339.53	−335.853	62.2827	−442.030	124.042		at 400 K
722	Chloromethane	C	−20.63	56.04	32.8153	2.44468	−9.69892	0.82007	0.11	0.354
		J	−86.32	234.47	137.299	10.2285	−40.5803	3.43118		at 400 K
723	Dichloromethane	C	−22.80	64.59	28.3856	4.11642	−35.6563	12.4875	0.54	1.229
		J	−95.40	270.24	118.765	17.2231	−149.186	52.2478		at 500 K
724	Chloroform	C	−24.20	70.66	57.3149	4.52075	−43.9598	15.8973	0.09	0.178
		J	−101.25	295.64	239 805	18.9148	−183.928	66.5143		at 400 K
725	Carbon tetrachloride	C	−24.00	74.12	97.2297	4.89180	−54.2024	21.1128	0.15	0.323
		J	−100.42	310.12	406.808	20.4673	−226.783	88.3358		at 400 K
726	Chloroethane	C	−26.70	65.93	8.99416	5.69633	−35.3404	8.95101	0.07	0,232
		J	−111.71	275.85	37.6316	23.8334	−147.864	37.4510		at 400 K
727	1,1-Dichloroethane	C	−31.05	72.89	29.7873	6.43770	−48.9499	15.0472	0.03	0.049
		J	−129.91	304.97	124.630	26.9353	−204.803	62.9576		at 400 K
728	1,2-Dichloroethane	C	−31.00	73.66	62.7788	5.17082	−34.7157	9.73220	0.12	0.327
		J	−129.70	308.19	262.666	21.6347	−145.250	40.7194		at 298 K
729	1,1,2-Trichloro-ethane	C	−33.10	80.57	44.2199	7.39755	−65.1156	22.1554	0.06	0.094
		J	−138.49	337.10	185.0158	30.9513	−272.444	92.6981		at 900 K
730	1,1,2,2-Tetra-chloroethane	C	−36.50	86.69	66.0162	7.76878	−71.0736	24.5654	0.06	0.111
		J	−152.72	362.71	276.211	32.5045	−297.372	102.782		at 900 K
731	Pentachloroethane	C	−34.00	90.95	104.268	8.09057	−80.6001	29.1697	0.07	0.129
		J	−142.26	380.53	436.256	33.8509	−337.231	122.046		at 500 K
732	Hexachloroethane	C	−33.80	94.77	146.253	8.50508	−93.4743	35.9598	0.15	0.330
		J	−141.42	396.52	611.923	35.5852	−391.096	150.456		at 400 K
733	1-Chloropropane	C	−31.10	76.20	0.28311	8.23190	−52.9932	14.2338	0.03	0.110
		J	−130.12	318.82	1.18452	34.4423	−221.724	59.5540		at 400 K
734	2-Chloropropane	C	−35.00	72.70	3.15597	8.37577	−54.0667	14.1414	0.09	0.319
		J	−146.44	304.18	13.2046	35.0442	−226.215	59.1675		at 400 K
735	1,2-Dichloro-propane	C	−39.60	84.80	24.7773	8.73757	−62.3097	18.5407	0.06	0.157
		J	−165.69	354.80	103.668	36.5579	−260.704	77.5740		at 400 K
736	1,3-Dichloro-propane	C	−38.60	87.76	42.5054	8.06204	−54.8370	15.4760	0.05	0.104
		J	−161.50	367.19	177.842	33.7315	−229.438	64.7513		at 500 K

Table I. (2. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
737	2,2-Dichloro-propane	C	−42.00	77.92	25.6438	9.79145	−80.5031	26.6027	0.05	0.083
		J	−175.73	326.02	107.293	40.9674	−336.825	111.306		at 500 K
738	1,2,3-Trichloro-propane	C	−44.40	91.52	64.1998	8.64914	−66.5441	20.9856	0.06	0.104
		J	−185.77	382.92	268.611	36.1879	−278.421	87.8036		at 500 K
739	1-Chlorobutane	C	−35.20	85.58	−2.11013	10.5126	−66.1682	17.1675	0.05	0.158
		J	−147.28	358.07	−8.82879	43.9847	−276.847	71.8288		at 400 K
740	Chlorobutane	C	−38.60	85.94	−0.40281	10.4934	−64.8301	16.5223	0.09	0.300
		J	−161.50	359.57	−1.68537	43.9043	−271.249	69.1295		at 400 K
741	1-Chloro-2-methylpropane	C	−38.10	84.56	−0.40281	10.4934	−64.8301	16.5223	0.09	0.300
		J	−159.41	353.80	−1.68537	43.9043	−271.249	69.1295		at 400 K
742	2-Chloro-2-methylpropane	C	−43.80	77.00	1.26241	11.2880	−80.1812	24.2105	0.08	0.134
		J	−183.26	322.17	5.28191	47.2289	−335.478	101.297		at 500 K
743	1-Chloropentane	C	−41.80	94.89	−4.50339	12.7933	−79.3432	20.1013	0.05	0.189
		J	−174.89	397.02	−18.8422	53.5272	−331.972	84.1037		at 400 K
744	1-Chloro-3-methylbutane	C	−43.10	95.56	−5.94292	13.3651	−89.1059	24.7528	0.08	0.232
		J	−180.33	399.82	−24.8652	55.9197	−372.819	103.566		at 400 K
745	2-Chloro-2-methylbutane	C	−48.40	88.06	−25.9002	13.9346	−92.1343	24.5029	0.16	0.438
		J	−202.51	368.44	−108.366	58.3023	−385.490	102.520		at 400 K
746	Chloroethylene	C	8.40	63.08	14.2107	4.82204	−36.6808	11.3950	0.04	0.082
		J	35.15	263.93	59.4575	20.1754	−153.472	47.6768		at 500 K
747	1,1-Dichloro-ethylene	C	0.30	68.85	35.3759	5.53156	−50.2098	17.6675	0.10	0.208
		J	1.26	288.07	148.013	23.1441	−210.078	73.9206		at 400 K
748	1,2-Dichloro-ethylene, cis	C	0.45	69.20	27.3389	5.6513	−50.4024	17.4122	0.07	0.113
		J	1.88	289.53	114.386	23.6401	−210.884	72.8525		at 400 K
749	1,2-Dichloro-ethylene, trans	C	1.00	69.29	43.4243	5.02632	−42.2929	13.9360	0.03	0.073
		J	4.18	289.91	181.687	21.0301	−176.953	58.3081		at 900 K
750	Trichloroethylene	C	−1.40	77.63	70.4336	5.46372	−52.0644	18.5548	0.09	0.205
		J	−5.86	324.80	294.694	22.8602	−217.837	77.6334		at 400 K
751	Tetrachloro-ethylene	C	−3.40	81.46	109.956	5.37880	−54.6679	19.9793	0.11	0.229
		J	−14.23	340.83	460.055	22.5049	−228.731	83.5934		at 400 K
752	3-Chloro-1-propene	C	−0.15	73.29	15.5932	6.79160	−46.6596	13.4936	0.03	0.068
		J	−0.63	306.65	65.2421	28.4161	−195.224	56.4572		at 900 K
753	Chlorobenzene	C	12.39	74.92	−74.1263	13.1307	−102.865	31.4567	0.06	0.147
		J	51.84	313.47	−310.144	54.9390	−430.386	131.615		at 400 K
754	o-Dichlorobenzene	C	7.16	81.61	−34.1551	13.1549	−107.839	34.1363	0.03	0.060
		J	29.96	341.46	−142.905	55.0402	−451.199	142,826		at 500 K
755	m-Dichloro-benzene	C	6.32	82.09	−32.4643	13.1181	−107.578	34.0768	0.04	0.078
		J	26.44	343.46	−135.831	54.8860	−450.107	142.577		at 500 K
756	p-Dichlorobenzene	C	5.50	80.47	−34.2623	13.2197	−108.874	34.5773	0.03	0.061
		J	23.01	336.69	−143.3533	55.3111	−455.531	144.671		at 500 K
757	Hexachloro-benzene	C	−8.10	105.45	130.031	12.9950	−123.172	42.5960	0.07	0.163
		J	−33.89	441.20	544.051	54.3711	−515.350	178.222		at 400 K
758	Acetyl chloride	C	−58.30	70.47	59.7472	4.08573	−23.5366	5.29938	0.05	0.164
		J	−243.93	294.85	249.982	17.0947	−98.4773	22.1726		at 400 K
759	Bromomethane	C	−9.00	58.75	34.4592	2.60621	−12.9015	2.38893	0.07	0.246
		J	−37.66	245.81	144.177	10.9044	−53.9797	9.99527		at 400 K
760	Bromoethane	C	−15.30	68.71	15.8969	5.60794	−35.1707	9.08486	0.09	0.240
		J	−64.02	287.48	66.5125	23.4636	−147.154	38.0110		at 400 K
761	1,2-Dibromo-ethane	C	−9.30	78.81	61.0916	5.94983	−42.8776	13.0744	0.09	0.230
		J	−38.91	329.74	255.607	24.8941	−179.400	54.7033		at 400 K

Table I. (3. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
762	1-Bromopropane	C	−21.00	79.08	7.83709	8.07521	−51.4658	13.6377	0.06	0.105
		J	−87.86	330.87	32.7904	33.7867	−215.333	57.0602		at 298 K
763	2-Bromopropane	C	−23.20	75.53	7.36662	8.38822	−55.2212	14.8531	0.09	0.245
		J	−97.07	316.02	30.8220	35.0963	−231.045	62.1455		at 400 K
764	1,2-Dibromo-propane	C	−17.40	89.90	31.5415	8.99470	−65.9457	19.5643	0.14	0.358
		J	−72.80	376.14	131.969	37.6338	−275.917	81.8570		at 300 K
765	1-Bromobutane	C	−25.65	88.39	5.44384	10.3559	−64.6408	16.5715	0.06	0.141
		J	−107.32	369.82	22.7770	43.3291	−270.457	69.3350		at 400 K
766	2-Bromobutane	C	−28.70	88.50	−0.07602	10.7588	−68.5968	17.9228	0.10	0.329
		J	−120.08	370.28	−0.31808	45.0148	−287.009	74.9890		at 400 K
767	2-Bromo-2-methyl-propane	C	−32.00	79.34	−21.0886	12.6448	−95.9709	29.3752	0.06	0.185
		J	−133.89	331.96	−88.2347	52.9057	−401.542	122.906		at 400 K
768	1,2-Dibromo-butane	C	−23.70	97.70	41.6592	10.8303	−75.0020	21.0276	0.08	0.170
		J	−99.17	408.78	174.302	45.3139	−313.808	87.9794		at 400 K
769	2,3-Dibromo-butane	C	−24.40	94.40	14.5573	11.8093	−85.1419	24.2999	0.07	0.136
		J	−102.09	394.97	60.9079	49.4103	−356.234	101.671		at 298 K
770	2,3-Dibromo-2-methylbutane	C	−33.20	98.60	−14.2313	15.5207	−115.964	34.0417	0.13	0.416
		J	−138.91	412.54	−59.5439	64.9386	−485.193	142.431		at 400 K
771	1-Bromopentane	C	−30.87	97.70	3.05060	12.6366	−77.8158	19.5052	0.06	0.175
		J	−129.16	408.78	12.7637	52.8716	−325.581	81.6099		at 400 K
772	Bromoethylene	C	18.73	65.83	21.5809	4.69485	−35.9252	11.2837	0.03	0.047
		J	78.37	275.43	90.2946	19.6433	−150.311	47.2109		at 500 K
773	3-Bromo-1-propene	C	11.80	75.80	15.9200	7.05702	−50.4262	14.8941	0.04	0.119
		J	49.37	317.15	66.6094	29.5266	−210.983	62.3168		at 298 K
774	Bromobenzene	C	25.10	77.53	−67.6393	12.7269	−96.7009	28.5929	0.06	0.201
		J	105.02	324.39	−283.003	53.2492	−404.596	119.633		at 400 K
775	Iodomethane	C	3.34	60.71	35.6318	2.79720	−16.5183	4.18004	0.04	0.134
		J	13.97	254.01	149.084	11.7035	−69.1126	17.4893		at 400 K
776	Diiodomethane	C	28.20	73.88	52.1573	4.78441	−33.5023	11.7548	0.08	0.117
		J	117.99	309.11	218.226	15.8341	−140.174	49.1822		at 700 K
777	Triiodomethane	C	50.40	85.00	99.3206	3.66242	−37.1390	13.9420	0.10	0.196
		J	210.87	355.64	415.557	15.3235	−155.390	58.3334		at 400 K
778	Iodoethane	C	−2.00	70.82	24.7596	5.35305	−32.6132	8.25378	0.03	0.095
		J	−8.37	296.31	103.594	22.3972	−136.453	34.5338		at 400 K
779	1,2-Diiodoethane	C	15.90	83.30	61.9069	5.61342	−40.2204	11.7395	0.05	0.116
		J	66.53	348.53	259.019	23.4866	−168.282	49.1170		at 500 K
780	1-Iodopropane	C	−7.30	80.32	28.8304	7.43082	−43.2015	10.0308	0.07	0.251
		J	−30.54	336.06	120.626	31.0906	−180.755	41.9687		at 400 K
781	2-Iodopropane	C	−10.00	77.55	11.6745	8.33443	−55.1031	14.9258	0.06	0.202
		J	−41.84	324.47	48.8461	34.8712	−230.551	62.4497		at 400 K
782	1,2-Diiodopropane	C	8.60	94.60	39.9343	8.65342	−61.9715	18.1561	0.04	0.097
		J	35.98	395.81	167.085	36.2059	−259.289	75.9652		at 500 K
783	2-Iodo-2-methyl-propane	C	−17.60	81.79	−12.6736	12.4545	−94.1225	28.7639	0.07	0.175
		J	−73.64	342.21	−53.0264	52.1095	−393.809	120.348		at 400 K
784	1,2-Diidobutane	C	2.85	101.80	55.2548	10.2662	−68.0983	18.4151	0.06	0.171
		J	11.92	425.93	231.186	42.9537	−284.923	77.0488		at 400 K
785	3-Iodo-1-propene	C	22.90	76.46	25.6768	7.25380	−54.9574	17.0669	0.07	0.214
		J	95.81	319.91	107.432	30.3499	−229.942	71.4079		at 700 K
786	Iodobenzene	C	38.85	79.84	−59.1881	12.7438	−98.9369	30.0247	0.06	0.155
		J	162.55	334.05	−247.643	53.3202	−413.952	125.624		at 400 K

Table I. (cont.)

ORGANIC SULFUR COMPOUNDS

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
800	Methyl sulfide	C	−8.97	68.32	54.3197	4.67884	−19.7073	2.64836	0.06	0.206
		J	−37.53	285.85	227.273	19.5763	−82.4553	11.0808		at 400 K
801	Ethyl methyl sulfide	C	−14.25	79.62	38.9456	7.31702	−35.6300	6.49051	0.07	0.241
		J	−59.62	333.13	162.948	30.6144	149.076	27.1563		at 400 K
802	Ethyl sulfide	C	−19.95	87.96	34.7078	9.43872	−43.3958	7.30327	0.09	0.287
		J	−83.47	368.02	145.217	39.4916	−181.568	30.5569		at 400 K
803	Isopropyl methyl sulfide	C	−21.61	85.87	32.5837	9.67742	−50.0188	12.2840	0.07	0.176
		J	−90.42	359.28	136.329	40.4903	−209.279	51.3965		at 400 K
804	Methyl propyl sulfide	C	−19.54	88.84	38.2843	9.36640	−44.1946	7.82698	0.07	0.241
		J	−81.76	371.71	160.182	39.1890	−184.910	32.7481		at 400 K
805	Butyl methyl sulfide	C	−24.42	98.43	44.2465	11.1682	−48.3067	7.26253	0.07	0.247
		J	−102.17	411.83	185.127	46.7277	−202.115	30.3864		at 400 K
806	Ethyl propyl sulfide	C	−25.00	98.97	37.5699	11.2405	−47.5080	6.73882	0.09	0.287
		J	−104.60	414.09	157.193	47.0303	−198.773	28.1952		at 400 K
807	Butyl ethyl sulfide	C	−29.92	108.27	34.3465	13.5641	−61.4125	10.0554	0.09	0.286
		J	−125.19	453.00	143.706	56.7523	−256.950	42.0718		at 400 K
808	Isopropyl sulfide	C	−33.76	99.30	−12.0193	17.3336	−123.815	36.9295	0.04	0.090
		J	−141.25	415.47	−50.2888	72.5238	−518.041	154.513		at 400 K
809	Methyl pentyl sulfide	C	−29.34	107.73	41.0230	13.4918	−62.2113	10.5791	0.08	0.252
		J	−122.76	450.74	171.640	56.4498	−260.292	44.2630		at 400 K
810	Propyl sulfide	C	−29.96	107.16	38.2280	13.1612	−53.4486	7.02146	0.10	0.321
		J	−125.35	448.36	159.946	55.0665	−223.629	29.3778		at 400 K
811	Butyl propyl sulfide	C	−34.88	117.90	37.2086	15.3659	−65.5247	9.49096	0.09	0.286
		J	−145.94	493.29	155.681	64.2911	−274.155	39.7102		at 400 K
812	Ethyl pentyl sulfide	C	−34.85	117.58	31.9532	15.8448	−74.5875	12.9892	0.09	0.292
		J	−145.81	491.95	133.692	66.2948	−312.074	54.3467		at 400 K
813	Hexyl methyl sulfide	C	−34.27	117.04	38.6298	15.7725	−75.3862	13.5129	0.08	0.262
		J	−143.39	489.70	161.627	65.9922	−315.416	56.5379		at 400 K
814	Butyl sulfide	C	−39.99	125.84	34.8154	17.6466	−78.6996	12.4247	0.09	0.291
		J	−167.32	526.51	145.667	73.8335	−329.279	51.9850		at 400 K
815	Ethyl hexyl sulfide	C	−39.77	126.89	28.7298	18.1685	−88.4920	16.3058	0.09	0.291
		J	−166.40	530.91	120.205	76.0168	−370.251	68.2233		at 400 K
816	Heptyl methyl sulfide	C	−39.19	126.35	35.4063	18.0961	−89.2912	16.8295	0.08	0.264
		J	−163.97	528.65	148.140	75.7142	−373.594	70.4145		at 400 K
817	Pentyl propyl sulfide	C	−39.81	127.21	34.8154	17.6466	−78.6993	12.4247	0.09	0.291
		J	−166.57	532.25	145.668	73.8334	−329.278	51.9849		at 400 K
818	Butyl pentyl sulfide	C	−44.92	136.52	31.5919	19.9703	−92.6042	15.7413	0.09	0.290
		J	−187.95	571.20	132.181	83.5555	−387.456	65.8616		at 400 K
819	Ethyl heptyl sulfide	C	−44.70	136.20	26.0912	20.4644	−101.956	19.4099	0.09	0.297
		J	−187.02	569.86	109.166	85.6229	−426.584	81.2110		at 400 K
820	Hexyl propyl sulfide	C	−44.73	136.52	31.5919	19.9703	−92.6042	15.7413	0.09	0.290
		J	−187.15	571.20	132.181	83.5555	−387.456	65.8616		at 400 K
821	Methyl octyl sulfide	C	−44.12	135.66	32.7678	20.3921	−102.755	19.9336	0.08	0.273
		J	−184.60	567.60	137.101	85.3204	−429.926	83.4022		at 400 K
822	Butyl hexyl sulfide	C	−49.84	145.83	28.9534	22.2662	−106.068	18.8454	0.09	0.296
		J	−208.53	610.15	121.141	93.1617	−443.790	78.8493		at 400 K

Table I. (1. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
823	Ethyl octyl sulfide	C	−49.63	145.51	22.9012	22.7866	−115.789	22.6661	0.09	0.303
		J	−207.65	608.81	95.8187	95.3393	−484.461	94.8349		at 400 K
824	Heptyl propyl sulfide	C	−49.66	145.83	28.9534	22,2661	−106.068	18.8454	0.09	0.295
		J	−207.78	610.15	121.141	93.1613	−443.788	78.8491		at 400 K
825	Methyl nonyl sulfide	C	−49.05	144.97	29.5778	22.7143	−116.587	23.1897	0.08	0.281
		J	−205.23	606.55	123.753	95.0363	−487.801	97.0257		at 400 K
826	Pentyl sulfide	C	−49.84	144.45	28.9534	22.2661	−106.068	18.8454	0.09	0.295
		J	−208.53	604.38	121.141	93.1613	−443.788	78.8491		at 400 K
827	Butyl heptyl sulfide	C	−54.77	155.14	25.7634	24.5884	−119.901	22.1016	0.09	0.301
		J	−229.16	649.11	107.794	102.878	−501.664	92.4729		at 400 K
828	Decyl methyl sulfide	C	−53.97	154.28	26.9406	25.0071	−129.984	26.2472	0.08	0.281
		J	−225.81	645.51	112.719	104.629	−543.854	109.818		at 400 K
829	Ethyl nonyl sulfide	C	−54.55	154.82	20.2640	25.0794	−129.185	25.7235	0.09	0.301
		J	−228.24	647.77	84.7843	104.932	−540.512	107.627		at 400 K
830	Octyl propyl sulfide	C	−54.56	155.14	25.7634	24.5884	−119.901	22.1016	0.09	0.301
		J	−228.28	649.11	107.794	102.878	−501.664	92.4729		at 400 K
831	Butyl octyl sulfide	C	−59.69	164.45	23.1262	26.8812	−133.298	25.1590	0.09	0.300
		J	−249.74	688.06	96.7595	112.471	−557.717	105.265		at 400 K
832	Decyl ethyl sulfide	C	−59.84	164.13	17.0393	27.4061	−143.157	29.0867	0.09	0.304
		J	−250.37	686.72	71.2921	114.667	−598.969	121.699		at 400 K
833	Hexyl sulfide	C	−59.69	163.07	23.1262	26.8812	−133.298	25.1590	0.09	0.300
		J	−249.74	682.28	96.7595	112.471	−557.717	105.265		at 400 K
834	Methyl undecyl sulfide	C	−58.90	163.59	23.7159	27.3338	−143.956	29.6104	0.09	0.286
		J	−246.44	684.46	99.2268	114.364	−602.311	123.890		at 400 K
835	Nonyl propyl sulfide	C	−59.51	164.45	23.1262	26.8812	−133.298	25.1590	0.09	0.300
		J	−248.99	688.06	96.7595	112.471	−557.717	105.265		at 400 K
836	Butyl nonyl sulfide	C	−64.62	173.76	19.9015	29.2079	−147.269	28.5223	0.09	0.300
		J	−270.37	727.01	83.2673	122.206	−616.174	119.337		at 400 K
837	Decyl propyl sulfide	C	−64.44	173.76	19.9015	29.2079	−147.269	28.5223	0.09	0.303
		J	−269.62	727.01	83.2673	122.206	−616.174	119.337		at 400 K
838	Dodecyl methyl sulfide	C	−63.82	172.90	22.2372	29.5616	−156.311	32.1585	0.08	0.275
		J	−267.02	723.41	93.0401	123.685	−654.003	134.551		at 400 K
839	Ethyl undecyl sulfide	C	−64.40	173.44	14.4021	29.6989	−156.554	32.1442	0.09	0.303
		J	−269.45	725.67	60.2579	124.260	−655.022	134.491		at 400 K
840	Butyl decyl sulfide	C	−69.55	183.07	17.2642	31.5007	−160.666	31.5797	0.09	0.302
		J	−291.00	765.96	72.2331	131.799	−672.227	132.129		at 400 K
841	Dodecyl ethyl sulfide	C	−69.33	182.75	11.4226	32.0104	−170.237	35.3371	0.09	0.305
		J	−290.08	764.63	47.7920	133.931	−712.269	147.850		at 400 K
842	Heptyl sulfide	C	−69.54	181.69	15.7926	31.5920	−162.401	32.6020	0.09	0.307
		J	−290.96	760.19	66.0759	132.181	−679.485	136.407		at 400 K
843	Methyl tridecyl sulfide	C	−68.75	182.21	18.0992	31.9381	−171.035	35.8608	0.09	0.289
		J	−287.65	762.37	75.7267	133.629	−715.611	150.041		at 400 K
844	Propyl undecyl sulfide	C	−69.36	183.07	17.2642	31.5007	−160.666	31.5797	0.09	0.302
		J	−290.20	765.96	72.2331	131.799	−672.227	132.129		at 400 K
845	Butyl undecyl sulfide	C	−74.47	192.38	14.2848	33.8122	−174.349	34.7726	0.09	0.304
		J	−311.58	804.92	59.7671	141.470	−729.474	145.488		at 400 K
846	Dodecyl propyl sulfide	C	−74.29	192.38	14.2848	33.8122	−174.349	34.7726	0.09	0.304
		J	−310.83	804.92	59.7671	141.470	−729.474	145.488		at 400 K

Table I. (2. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
847	Ethyl tridecyl sulfide	C	−74.26	192.06	8.29914	34.3341	−184.141	38.6537	0.09	0.304
		J	−310.71	803.58	34.7235	143.653	−770.446	161.727	at 400 K	
848	Methyl tetradecyl sulfide	C	−73.68	191.52	14.9757	34.2617	−184.940	39.1774	0.09	0.288
		J	−308.28	801.32	62.6582	143.351	−773.788	163.918	at 400 K	
849	Butyl dodecyl sulfide	C	−79.40	201.69	11.1613	36.1359	−188.253	38.0892	0.09	0.302
		J	−332.21	843.87	46.6987	151.192	−787.651	159.365	at 400 K	
850	Ethyl tetradecyl sulfide	C	−79.18	201.36	5.07568	36.6577	−198.046	41.9703	0.09	0.302
		J	−331.29	842.49	21.2366	153.375	−828.623	175.603	at 400 K	
851	Methyl pentadecyl sulfide	C	−78.60	200.82	11.7523	36.5854	−198.845	42.4940	0.09	0.288
		J	−328.86	840.23	49.1713	153.073	−831.964	177.794	at 400 K	
852	Octyl sulfide	C	−79.39	200.31	11.1613	36.1359	−188.253	38.0892	0.09	0.302
		J	−332.17	838.10	46.6987	151.192	−787.651	159.365	at 400 K	
853	Propyl tridecyl sulfide	C	−79.22	201.69	11.1613	36.1359	−188.253	38.0892	0.09	0.302
		J	−331.46	843.87	46.6987	151.192	−787.651	159.365	at 400 K	
854	Butyl tridecyl sulfide	C	−84.32	210.99	7.93783	38.4595	−202.158	41.4058	0.09	0.301
		J	−352.79	882.78	33.2118	160.914	−845.827	173.241	at 400 K	
855	Ethyl pentadecyl sulfide	C	−84.11	210.67	2.68242	38.9384	−211.221	44.9041	0.09	0.304
		J	−351.92	881.44	11.2232	162.918	−883.748	187.878	at 400 K	
856	Hexadecyl methyl sulfide	C	−83.53	210.13	9.35898	38.8661	−212.020	45.4280	0.09	0.291
		J	−349.49	879.18	39.1580	162.616	−887.092	190.071	at 400 K	
857	Propyl tetradecyl sulfide	C	−84.14	210.99	7.93783	38.4595	−202.158	41.4058	0.09	0.301
		J	−352.04	882.78	33.2118	160.914	−845.827	173.241	at 400 K	
858	Butyl tetradecyl sulfide	C	−89.25	220.30	5.54458	40.7402	−215.333	44.3396	0.09	0.303
		J	−373.42	921.74	23.1985	170.456	−900.951	185.516	at 400 K	
859	Ethyl hexadecyl sulfide	C	−89.03	219.98	−0.54104	41.2620	−225.126	48.2207	0.09	0.303
		J	−372.50	920.40	−2.26372	172.640	−941.926	201.755	at 400 K	
860	Heptadecyl methyl sulfide	C	−88.45	219.44	6.13553	41.1897	−225.925	48.7446	0.09	0.290
		J	−370.07	918.14	25.6711	172.338	−945.268	203.947	at 400 K	
861	Nonyl sulfide	C	−89.25	218.92	5.54455	40.7402	−215.333	44.3398	0.09	0.303
		J	−373.42	915.96	23.1984	170.457	−900.955	185.518	at 400 K	
862	Pentadecyl propyl sulfide	C	−89.07	220.30	5.54455	40.7402	−215.333	44.3398	0.09	0.303
		J	−372.67	921.74	23.1984	170.457	−900.955	185.518	at 400 K	
863	Butyl pentadecyl sulfide	C	−94.18	229.61	−39.7951	45.2155	−259.299	60.3121	0.29	0.843
		J	−394.05	960.69	−166.503	189.181	−1084.91	252.345	at 600 K	
864	Ethyl heptadecyl sulfide	C	−93.96	229.29	−3.17955	43.5580	−238.590	51.3248	0.09	0.305
		J	−393.13	959.35	−13.3032	182.246	−998.259	214.743	at 400 K	
865	Hexadecyl propyl sulfide	C	−93.99	229.61	2.32110	43.0638	−229.238	47.6564	0.09	0.302
		J	−393.25	960.69	9.71149	180.179	−959.131	199.394	at 400 K	
866	Methyl octadecyl sulfide	C	−93.38	228.75	3.49701	43.4856	−239.389	51.8487	0.09	0.293
		J	−390.70	957.09	14.6315	181.944	−1001.60	216.935	at 400 K	
867	Butyl hexadecyl sulfide	C	−99.10	238.92	−0.31741	45.3598	−242.702	50.7606	0.09	0.304
		J	−414.63	999.64	−1.32806	189.785	−1015.47	212.382	at 400 K	
868	Decyl sulfide	C	−99.10	237.54	−0.31741	45.3598	−242.702	50.7606	0.09	0.304
		J	−414.63	993.87	−1.32806	189.785	−1015.47	212.382	at 400 K	
869	Ethyl octadecyl sulfide	C	−98.89	238.60	−6.36962	45.8802	−252.424	54.5810	0.09	0.308
		J	−413.76	998.30	−26.6505	191.963	−1056.14	228.367	at 400 K	
870	Heptadecyl propyl sulfide	C	−98.92	238.92	−0.31741	45.3598	−242.702	50.7604	0.09	0.304
		J	−413.88	999.64	−1.32806	189.785	−1015.47	212.382	at 400 K	

Table I. (3. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
871	Methyl nonadecyl sulfide	C	−98.31	238.06	0.30698	45.8079	−253.221	55.1047	0.09	0.296
		J	−411.33	996.04	1.28440	191.660	−1059.48	230.558		at 400 K
872	Methyl disulfide	C	−5.77	80.46	83.5808	5.50682	−26.6308	4.49777	0.07	0.198
		J	−24.14	336.64	349.702	23.0405	−111.423	18.8187		at 700 K
873	Ethyl disulfide	C	−17.84	99.07	53.8044	11.5500	−73.7162	18.7899	0.07	0.215
		J	−74.64	414.51	225.118	48.3250	−308.428	78.6168		at 400 K
874	Propyl disulfide	C	−28.01	118.30	54.3904	15.4122	−85.7186	19.3354	0.07	0.202
		J	−117.19	494.97	227.569	64.4847	−358.647	80.8993		at 400 K
875	Butyl disulfide	C	−37.86	136.91	48.7737	20.0165	−112.798	25.5858	0.07	0.224
		J	−158.41	572.83	204.069	83.7492	−471.947	107.051		at 400 K
876	Pentyl disulfide	C	−47.71	155.53	42.9118	24.6360	−140.166	32.0064	0.08	0.239
		J	−199.62	650.74	179.543	103.077	−586.455	133.915		at 400 K
877	Hexyl disulfide	C	−57.56	174.15	37.0845	29.2511	−167.396	38.3200	0.08	0.251
		J	−240.83	728.64	155.162	122.387	−700.384	160.331		at 400 K
878	Heptyl disulfide	C	−67.41	192.77	31.2226	33.8706	−194.764	44.7407	0.08	0.259
		J	−282.04	806.55	130.635	141.715	−814.894	187.195		at 400 K
879	Octyl disulfide	C	−77.27	211.39	25.1197	38.5057	−222.351	51.2502	0.08	0.264
		J	−323.30	884.46	105.101	161.108	−930.318	214.431		at 400 K
880	Nonyl disulfide	C	−87.12	230.00	19.5029	43.1101	−249.432	57.5007	0.08	0.269
		J	−364.51	962.32	−81.6003	180.373	−1043.62	240.583		at 400 K
881	Decyl disulfide	C	−96.97	248.62	13.6410	47.7297	−276.800	63.9214	0.08	0.273
		J	−405.72	1040.23	57.0738	199.701	−1158.13	267.447		at 400 K
882	Thiacyclopropane	C	−19.65	61.01	−28.4667	6.65125	−51.5224	16.0774	0.06	0.109
		J	−82.22	255.27	−119.105	27.8288	−215.570	67.2679		at 500 K
883	Thiacyclobutane	C	14.61	68.17	−46.6570	8.60408	−53.8486	13.1260	0.12	0.386
		J	61.13	285.22	−195.213	35.9995	−225.303	54.9193		at 400 K
884	Thiacyclopentane	C	−8.08	73.94	−79.4323	12.3147	−86.8658	24.7955	0.05	0.107
		J	−33.81	309.36	−332.345	51.5248	−363.446	103.745		at 298 K
885	Thiacyclohexane	C	−15.12	77.26	−124.354	15.1059	−80.9204	14.5664	0.23	0.732
		J	−63.26	323.26	−520.298	63.2033	−338.571	60.9459		at 400 K
886	Thiacycloheptane	C	−14.66	86.50	−168.546	17.3952	−57.6233	−11.7768	0.74	0.764
		J	−61.34	361.92	−705.195	72.7815	−241.096	−49.2743		at 298 K
887	Thiophene	C	27.66	66.65	−71.0359	10.6014	−88.3326	28.9751	0.05	0.102
		J	115.73	278.86	−297.214	44.3562	−369.584	121.232		at 500 K
888	2-Methylthiophene	C	20.00	76.62	−45.6756	11.3896	−81.1596	23.1272	0.05	0.188
		J	83.68	320.58	−191.107	47.6539	−339.572	96.7642		at 400 K
889	3-Methylthiophene	C	19.79	76.79	−55.2854	11.9006	−90.0250	27.1458	0.05	0.093
		J	82.80	321.29	−231.314	49.7922	−376.665	113.578		at 400 K
890	Methanethiol	C	−5.49	60.96	47.0575	2.77850	−11.5313	1.51163	0.07	0.224
		J	−22.97	255.06	196.888	11.6253	−48.2470	6.32465		at 400 K
891	Ethanethiol	C	−11.02	70.77	33.7507	5.52522	−29.9366	6.68050	0.05	0.159
		J	−46.11	296.10	141.213	23.1175	−125.255	27.9512		at 400 K
892	1-Propanethiol	C	−16.22	80.40	36.6129	7.32701	−34.0487	6.11605	0.06	0.190
		J	−67.86	336.39	153.188	30.6562	−142.460	25.5896		at 400 K
893	2-Propanethiol	C	−18.22	77.51	15.8720	8.65177	−54.3025	14.1078	0.06	0.207
		J	−76.23	324.30	66.4085	36.1990	−227.201	59.0268		at 400 K
894	1-Butanethiol	C	−21.05	89.68	42.5750	9.12881	−38.1608	5.55161	0.06	0.206
		J	−88.07	375.22	178.134	38.1949	−159.665	23.2279		at 400 K

Table 1. (4. cont.)

No.	Compound		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
895	2-Butanethiol	C	−23.00	87.65	15.5563	10.8667	−66.1510	15.9335	0.07	0.220
		J	−96.23	366.73	65.0876	45.4662	−276.776	66.6660		at 400 K
896	2-Methyl-1-propanethiol	C	−23.24	86.73	−3.25494	11.7934	−80.4798	22.0317	0.06	0.201
		J	−97.24	362.88	−13.6187	49.3434	−336.727	92.1805		at 400 K
897	2-Methyl-2-propanethiol	C	−26.17	80.79	−1.15918	11.8434	−76.8318	19.7358	0.08	0.270
		J	−109.50	338.03	−4.85002	49.5529	−321.464	82.5746		at 400 K
898	2-Methyl-2-butanethiol	C	−30.36	92.48	8.34674	13.4673	−81.1805	18.9417	0.10	0.320
		J	−127.03	386.94	34.9228	56.3473	−339.659	79.2521		at 400 K
899	1-Pentanethiol	C	−25.91	99.28	40.3011	11.4266	−51.6485	8.65565	0.07	0.230
		J	−108.41	415.39	168.620	47.8090	−216.097	36.2152		at 400 K
900	1-Hexanethiol	C	−30.83	108.58	37.0776	13.7502	−65.5531	11.9722	0.07	0.238
		J	−128.99	454.30	155.133	57.5310	−274.274	50.0918		at 400 K
901	1-Heptanethiol	C	−35.76	117.89	34.6844	16.0309	−78.7281	14.9060	0.07	0.250
		J	−149.62	493.25	145.119	67.0735	−329.398	62.3667		at 400 K
902	1-Octanethiol	C	−40.68	127.20	31.4609	18.3546	−92.6326	18.2226	0.08	0.253
		J	−170.21	532.20	131.633	76.7955	−387.575	76.2433		at 400 K
903	1-Nonanethiol	C	−45.61	136.51	28.8224	20.6505	−106.097	21.3267	0.08	0.263
		J	−190.83	571.16	120.593	86.4016	−443.909	89.2310		at 400 K
904	1-Decanethiol	C	−50.54	145.82	25.6324	22.9727	−119.930	24.5829	0.08	0.272
		J	−211.46	610.11	107.2459	96.1179	−501.785	102.855		at 400 K
905	1-Undecanethiol	C	−55.46	155.13	22.9951	25.2656	−133.327	27.6403	0.08	0.273
		J	−232.04	649.06	96.2117	105.711	−557.838	115.647		at 400 K
906	1-Dodecanethiol	C	−60.39	164.44	19.7704	27.5923	−147.298	31.0036	0.08	0.278
		J	−252.67	688.02	82.7194	115.446	−616.296	129.719		at 400 K
907	1-Tridecanethiol	C	−65.31	173.75	17.1332	29.8851	−160.695	34.0611	0.08	0.279
		J	−273.26	726.97	71.6852	125.039	−672.348	142.512		at 400 K
908	1-Tetradecanethiol	C	−70.24	183.06	14.1537	32.1966	−174.378	37.2540	0.08	0.282
		J	−293.88	765.92	59.2192	13.4711	−729.596	155.871		at 400 K
909	1-Pentadecanethiol	C	−75.17	192.37	11.0303	34.5202	−188.282	40.5706	0.08	0.282
		J	−314.51	804.88	46.1507	144.433	−787.773	169.747		at 400 K
910	1-Hexadecanethiol	C	−80.09	201.67	7.80682	36.8438	−202.187	43.8872	0.08	0.282
		J	−335.10	843.79	32.6637	154.155	−845.950	183.624		at 400 K
911	1-Heptadecanethiol	C	−85.02	210.98	5.41357	39.1245	−215.362	46.8209	0.08	0.285
		J	−355.72	882.74	22.6504	163.697	−901.074	195.899		at 400 K
912	1-Octadecanethiol	C	−89.94	220.29	2.19012	41.4481	−229.266	50.1375	0.08	0.285
		J	−376.31	921.69	9.16348	173.419	−959.250	209.775		at 400 K
913	1-Nonadecanethiol	C	−94.87	229.60	2.78306	43.5977	−240.629	52.2770	0.09	0.297
		J	−396.94	960.65	11.6443	182.413	−1006.79	218.727		at 400 K
914	Eicosanethiol	C	−99.80	238.91	−3.63843	46.0663	−256.563	56.4978	0.09	0.292
		J	−417.56	999.60	−15.2232	192.741	−1073.46	236.387		at 400 K
915	Cyclopentanethiol	C	−11.45	86.38	−86.9286	13.9016	−84.7170	20.2109	0.10	0.354
		J	−47.91	361.41	−363.709	58.1645	−354.456	84.5624		at 400 K
916	Benzenethiol	C	26.66	80.51	−74.9482	13.7858	−105.622	32.0540	0.05	0.123
		J	111.55	336.85	−313.583	57.6799	−441.927	134.114		at 400 K
917	Isothiocyanic acid	C	30.50	59.28	35.3143	3.46105	−34.9145	13.3656	0.20	0.516
		J	127.61	248.03	147.755	14.4810	−146.082	55.9215		at 400 K
918	Thioacetic acid	C	−43.49	74.86	91.9370	3.89759	−16.7405	1.14629	0.23	0.537
		J	−181.96	313.21	384.665	16.3075	−70.0424	4.79610		at 700 K

Table I. (cont.)

FREE RADICALS

No.	Radical		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
1001	$CH_3^\bullet$	C	34.0	46.4	60.3536	0.61738	5.54378	−3.75381	0.26	0.608
		J	142.3	194.1	252.520	2.58313	23.1952	−15.7059		at 500 K
1002	$C_2H_5^\bullet$	C	25.7	59.5	−0.03838	4.67829	−29.3463	8.47246	0.13	0.301
		J	107.5	248.9	−0.16057	19.5740	−122.785	35.4488		at 400 K
1003	$n-C_3H_7^\bullet$	C	20.7	68.1	17.4997	6.24272	−33.4701	7.58098	0.19	0.366
		J	86.6	284.9	73.2189	26.1196	−140.039	31.7188		at 600 K
1004	$i-C_3H_7^\bullet$	C	17.6	67.0	36.5238	5.19485	−19.9818	2.17358	0.17	0.413
		J	73.6	280.3	152.816	21.7353	−83.6038	9.09427		at 500 K
1005	$CH_3\dot{C}HCH_2CH_3$	C	2.3	77.6	37.0702	7.27014	−27.6785	1.55819	0.14	0.265
		J	9.6	324.7	155.102	30.4183	−115.807	6.51945		at 600 K
1006	$(CH_3)_3C^\bullet$	C	8.9	72.2	0.55392	6.96961	−17.0626	−3.79718	0.37	0.870
		J	37.2	302.1	2.31760	29.1608	−71.3899	−15.8874		at 500 K
1007	$\emptyset^\bullet$	C	80.0	69.1	−89.1977	11.6246	−84.9627	24.3985	0.02	0.055
		J	334.7	289.1	−373.203	48.6372	−355.484	102.083		at 400 K
1008	$\emptyset CH_2^\bullet$	C	45.0	75.4	−79.2028	13.7134	−95.7835	26.4695	0.15	0.367
		J	188.3	315.5	−331.384	57.3770	−400.758	110.748		at 400 K
1009	$\emptyset\dot{C}HCH_3$	C	36.6	85.1	−85.9307	15.9819	−107.707	28.2797	0.12	0.260
		J	153.1	356.1	−359.534	66.8683	−450.644	118.322		at 500 K
1010	$\emptyset O^\bullet$	C	19.5	73.7	−99.0662	13.8135	−111.034	35.1033	0.04	0.095
		J	81.6	308.4	−414.493	57.7955	−464.567	146.872		at 400 K
1011	$\emptyset S^\bullet$	C	49.5	76.5	−70.8897	12.9128	−98.2763	28.5316	0.09	0.208
		J	207.1	320.1	−296.603	54.0270	−411.188	119.376		at 400 K
1012	$\emptyset\dot{C}(CH_3)_2$	C	26.3	90.6	−45.7918	16.0172	−89.2669	17.3478	0.21	0.469
		J	110.0	379.1	−191.593	67.0159	−373.493	72.5833		at 400 K
1013	$CH_3S^\bullet$	C	28.0	57.6	41.1623	2.04837	−4.24743	−1.55349	0.99	2.274
		J	117.2	241.0	172.223	8.57036	−17.7712	−6.49980		at 500 K
1014	$CH_3CH_2S^\bullet$	C	22.3[a]	67.2	22.1283	4.99504	−24.2188	4.24309	0.39	1.02
		J	93.4	281.2	92.5847	20.8993	−101.332	17.7531		at 400 K
1015	$(CH_3)_2CHS^\bullet$	C	15.3	74.2	8.35534	8.04106	−49.4003	12.2476	0.29	0.694
		J	64.2	310.5	34.9587	33.6438	−206.691	51.2439		at 400 K
1016	$(CH_3)_3CS^\bullet$	C	7.3[a]	77.2	−17.7325	11.7623	−82.6916	23.4183	0.31	0.728
		J	30.4	323.0	−74.1929	49.2135	−345.981	97.9823		at 400 K
1017	$CH_3O^\bullet$	C	3.9	54.3	32.3550	2.00044	−1.17211	−3.17925	0.56	1.321
		J	16.3	227.2	135.248	8.36983	−4.90410	−13.3020		at 400 K
1018	$CH_3CH_2O^\bullet$	C	4.9	64.6	33.8226	3.69938	−1.63848	−7.54882	0.67	1.588
		J	20.5	270.3	141.514	15.4782	−6.85540	−31.5843		at 500 K
1019	$(CH_3)_2CHO^\bullet$	C	−6.69	71.1	14.5989	7.13127	−31.3451	2.56060	0.28	0.676
		J	−28.0	297.5	61.0817	29.8372	−131.148	10.7136		at 500 K
1020	$(CH_3)_3CO^\bullet$	C	−21.5	75.0	11.0459	9.54936	−45.0195	5.01243	0.36	0.845
		J	−90.0	313.8	46.2161	39.9545	−188.362	20.9720		at 500 K
1021	$CH_2=CHCH_2^\bullet$	C	39.6	62.1	−13.2380	6.56231	−45.5646	13.1745	0.18	0.378
		J	165.7	259.8	−55.3878	27.4567	−190.642	55.1220		at 600 K
1022	$CH_2=C(CH_3)CH_2^\bullet$	C	29.6	68.8	−11.0347	9.10765	−66.1467	20.5824	0.11	0.221
		J	123.8	287.9	−46.1691	38.1064	−276.758	86.1166		at 600 K
1023	$CH_2=CH\dot{C}HCH_3$	C	30.4	70.8	−15.4190	8.74819	−56.5500	14.9133	0.07	0.168
		J	127.2	296.2	−64.5129	36.6024	−236.605	62.3974		at 400 K

Table I. (1. cont.)

No.	Radical		ΔH_f° 298 K	S° 298 K	$a \cdot 10$	$b \cdot 10^2$	$c \cdot 10^6$	$d \cdot 10^9$	Av. err. %	Max. rel. err. %
024	$CH_3CO\dot{2}$	C	−49.7	66.6	62.7632	2.23532	−2.44894	−2.88438	0.12	0.281
		J	−207.9	278.7	262.601	9.35260	−10.2464	−12.0682		at 400 K
1025	$CH_3CH_2CO\dot{2}$	C	−55.0	76.2	66.3594	4.75244	−23.1130	4.46461	0.18	0.339
		J	−230.1	318.8	277.648	19.8842	−96.7050	18.6799		at 600 K
1026	$NH\dot{2}$	C	41.0	48.4	50.1229	1.45866	−17.4743	9.46511	0.44	0.862
		J	171.5	202.5	209.714	6.10305	−73.1125	39.6020		at 600 K
1027	$\dot{C}H_2C{\equiv}N$	C	51.1	58.5	16.8955	3.82508	−30.3805	10.2424	0.06	0.121
		J	213.8	244.8	70.6907	16.0041	−127.112	42.8542		at 400 K
1028	$CH_3\dot{C}HC{\equiv}N$	C	42.72[a]	68.8	−0.81586	6.30949	−42.7553	11.6441	0.08	0.206
		J	178.7	287.9	−3.41355	26.3989	−178.888	48.7190		at 400 K
1029	$(CH_3)_2\dot{C}{-}C{\equiv}N$	C	33.8	75.8	64.1754	5.44520	−16.1227	−1.24778	0.53	1.212
		J	141.4	317.1	268.510	22.7827	−67.4573	−5.22070		at 500 K
1030	$CH_3\dot{N}H$	C	34.9	59.0	39.1535	2.81741	−12.6148	2.22128	0.11	0.249
		J	146.0	246.9	163.818	11.7880	−52.7803	9.29385		at 600 K
1031	$(CH_3)_2\dot{N}$	C	31.9	66.2	21.7546	5.12302	−21.9637	2.84355	0.30	0.700
		J	133.5	277.0	91.0212	21.4347	−91.8961	11.8974		at 400 K
1032	$\emptyset\dot{N}H$	C	47.3	75.3	−112.809	15.5828	−131.384	43.1410	0.04	0.081
		J	197.9	315.1	−471.994	65.1983	−549.711	180.502		at 600 K
1033	$\emptyset\dot{N}CH_3$	C	48.6	83.3	−85.7191	16.1242	−116.862	33.1859	0.06	0.130
		J	203.3	348.5	−358.649	67.4637	−488.949	138.850		at 400 K
1034	$\dot{C}OOH$	C	−53.3	60.7	42.4427	2.49971	−18.0493	5.12770	0.59	1.100
		J	−223.0	254.0	177.580	10.4588	−75.5183	21.4543		at 600 K
1035	$(CH_3)_3C\dot{C}H_2$	C	7.1[a]	78.8	61.6004	6.62492	34.4757	−42.9253	0.54	1.048
		J	29.7	329.7	257.736	27.7187	144.246	−179.599		at 400 K
1036	$CH_3\dot{C}HCH(CH_3)_2$	C	5.3[a]	84.7	14.9877	10.3417	−52.7143	10.2847	0.13	0.255
		J	22.2	354.4	62.7086	43.2695	−220.557	43.0311		at 400 K

[a]) Calculated from the group additivity values of ref. [11].

[b]) Calculated from data in ref [12]. Since the C_p^0 values in ref. [10] and ref. [12] are slightly different, the correlation cofficients are also different.

The enthalpy increments between 298 and 800 K were calculated from both sets of correlation constants and compared with the experimental data for a number of compounds (Table III). The improvement in the calculated values is marked in most cases. For this reason, the correlation constants compiled in Table I should be preferred when the calculation of thermodynamic functions is to be performed in the temperature range of 298—1000 K.

Since the data collected in Table I are based on C_p^0 values between 298 and 1000 K, they are not applicable at considerably higher temperatures. However, as can be judged from the data of Table IV, extrapolations up to 1100 K are allowed without an important increase in the error of calculation.

Table II.

The improvement of heat capacity prediction by decreasing the temperature range of calculation of correlation constans of eq. (3).[a])

Compound	Temp. range K	a	$b \cdot 10^3$	$c \cdot 10^6$	$d \cdot 10^9$	Max. rel. err. %
Carbon dioxide	298—1000	19.7352	73.7457	−56.8008	17.7092	0.15 at 400 K
	298—1500	21.5238	63.8891	−40.7492	9.75347	0.38 at 400 K
Methane	298—1000	24.9065	19.7660	67.1427	−39.9065	0.64 at 400 K
	298—1500	17.8571	58.8245	3.07692	−7.89514	1.53 at 400 K
Acetylene	298—1000	15.8398	128.050	−127.788	50.6153	0.49 at 400 K
	298—1500	23.4733	85.7216	−58.2873	15.8497	1.31 at 400 K
Propene	298—1000	5.09112	225.513	−99.6863	13.2019	0.35 at 400 K
	298—1500	3.25367	236.086	−117.883	22.7792	0.47 at 400 K
1,3-Butadiene	298—1000	−16.1192	412.161	−340.122	113.673	0.13 at 500 K
	298—1500	−2.89908	339.772	−223.279	56.3757	0.92 at 500 K
c-Hexane	298—1000	−55.3308	617.495	−261.029	15.6487	0.67 at 400 K
	298—1500	−67.6047	687.584	−380.544	77.952	1.08 at 400 K
Benzene	298—1000	−43.7404	522.853	−375.335	106.086	0.21 at 400 K
	298—1500	−35.8988	480.836	−309.542	74.9846	0.51 at 500 K

[a]) C_p^0 in J mol^{-1} K^{-1}

Table III

The improvement of enthalpy calculation by decreasing the temperature range of calculation of correlation constants

Compound	A kJ mol^{-1}	B kJ mol^{-1}	Rel. err. of B %	C kJ mol^{-1}	Rel. err. of C %
Carbon dioxide	22.97	22.79	0.78	22.81	0.70
Methane	24.74	24.88	0.57	24.80	0.24
Acetylene	27.65	27.56	0.33	27.64	0.04
Propene	49.84	49.90	0.12	49.89	0.10
1,3-Butadiene	61.85	61.70	0.24	61.86	0.02
c-Hexane	101.63	101.8	0.17	101.7	0.07
Benzene	72.01	71.92	0.12	72.04	0.04

A: experimental value of $\int_{298}^{800} Cp\, dT$ [12]

B: calculated value of the above integral (constants derived for the temperature range 298—1500 K)

C: calculated value of the above integral (constants derived for the temperature range 298—1000 K).

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Table IV

Extrapolations to higher temperatures

Compound	C_p^0 at 1100 K J mol^{-1} K^{-1} exp.	calc.	C_p^0 at 1200 K J mol^{-1} K^{-1} exp.	calc.	Rel. err. at 1100 K %	Rel. err. at 1200 K %
Carbon dioxide	55.48	55.70	56.44	57.04	0.40	1.06
Methane	75.70	74.75	79.0	76.35	1.25	3.35
Acetylene	68.42	69.44	70.06	72.95	1.01	1.04
Propene	150.6	150.11	156.1	154.97	0.33	0.72
1,3-Butadiene	175.8	175.72	181.3	180.72	0.05	0.32
c-Hexane	331.8	328.90	343.9	336.87	0.87	2.04
Benzene	218.2	218.44	225.4	226.52	0.11	0.50

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БОЛЕЕ ТОЧНОЕ ОПРЕДЕЛЕНИЕ МОЛЯРНЫХ ТЕПЛОЕМКОСТЕЙ

Л. Шереш, Л. Залотаи и Ф. Марта

Сведения о теплоемкостях химических соединений весьма важны как при научных экспериментах, так и при проектировании промышленных производств. В работе приведены теплоемкости более чем 700 соединений с относительной ошибкой не превышающей 0,1% для интервала температур от 273 до 1000 К, на основании кривых рассчитанных с использованием полинома:

$$C_p^0 = a + bT + cT^2 + dT^3.$$

Полученные кривые хорошо удовлетворяют экспериментальным значениям C_p^0. Представленные данные выражены как в единицах калории, так и в джоулях.